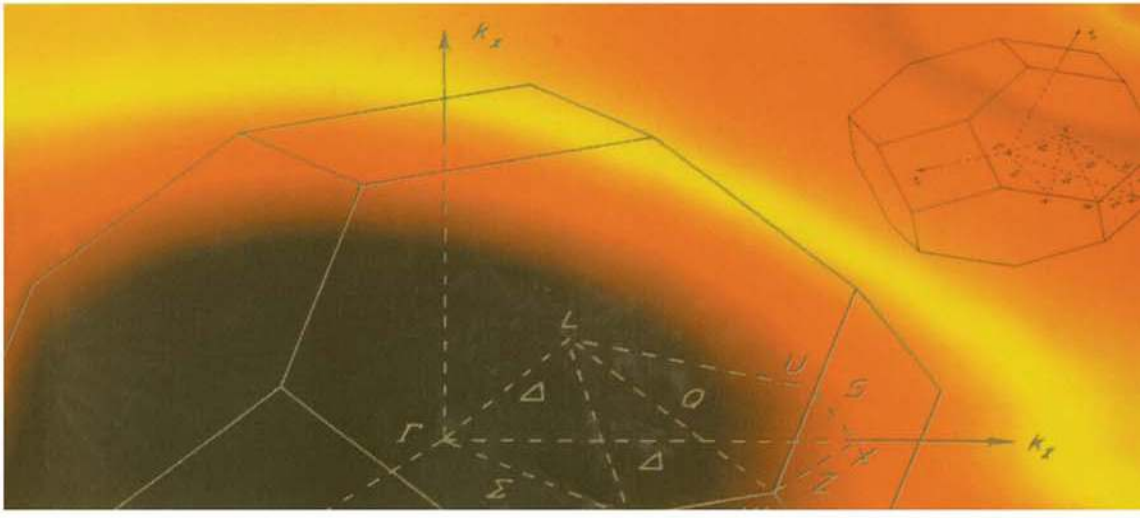
GROUP THEORY IN PHYSICS



AN INTRODUCTION

J. F. CORNWELL

Group Theory in Physics

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Preface

As was observed previously in the preface to my three-volume work *Group Theory in Physics*, thirty years or so ago group theory could have been regarded by physicists as merely providing a very valuable tool for the elucidation of the symmetry aspects of physical problems. However, recent developments, particularly in high-energy physics, have transformed its role, so that it now occupies a crucial and indispensable position at the centre of the stage. These developments have taken physicists increasingly deeper into the fascinating world of the pure mathematicians, and have led to an ever-growing appreciation of their achievements, the full recognition of which has been hampered to some extent by the style in which much of modern pure mathematics is presented. As with my previous three-volume treatise, one of the main objectives of the present work is to try to overcome this communication barrier, and to present to theoretical physicists and others some of the important mathematical developments in a form that should be easier to comprehend and appreciate.

Although my *Group Theory in Physics* was intended to provide a introduction to the subject, it also aimed to provide a thorough and self-contained account, and so its overall length may well have made it appear rather daunting. The present book has accordingly been designed to provide a much more succinct introduction to the subject, suitable for advanced undergraduate and postgraduate students, and for others approaching the subject for the first time. The treatment starts with the basic concepts and is carried through to some of the most significant developments in atomic physics, electronic energy bands in solids, and the theory of elementary particles. No prior knowledge of group theory is assumed, and, for convenience, various relevant algebraic concepts are summarized in Appendices A and B.

The present work is essentially an abridgement of Volumes I and II of *Group Theory in Physics* (which hereafter will be referred to as "Cornwell (1984)"), although some new material has been included. The intention has been to concentrate on introducing and describing in detail the most important basic ideas and the role that they play in physical problems. Inevitably restrictions on length have meant that some other important concepts and developments have had to be omitted. Nevertheless the mathematical coverage goes outside the strict confines of group theory itself, for one soon is led to the study of Lie algebras, which, although related to Lie groups, are often

developed by mathematicians as a separate subject.

Mathematical proofs have been included only when the direct nature of their arguments assist in the appreciation of theorems to which they refer. In other cases references have been given to works in which they may be found. In many instances these references are quoted as "Cornwell (1984)", as interested readers may find it useful to see these proofs with the same notations, conventions, and nomenclature as in the present work. Of course, this is *not* intended to imply that this reference is either the original source or the only place in which a proof may be found. The same reservation naturally applies to the references to suggested further reading on topics that have been explicitly omitted here.

In the text the treatments of specific cases are frequently given under the heading of "Examples". The format is such that these are clearly distinguished from the main part of the text, the intention being that to indicate that the detailed analysis in the Example is not essential for the general understanding of the rest of that section or the succeeding sections. Nevertheless, the Examples are important for two reasons. Firstly, they give concrete realizations of the concepts that have just been introduced. Secondly, they indicate how the concepts apply to certain physically important groups or algebras, thereby allowing a "parallel" treatment of a number of specific cases. For instance, many of the properties of the groups SU(2) and SU(3) are developed in a series of such Examples.

For the benefit of readers who may wish to concentrate on specific applications, the following list gives the relevant chapters:

(i) electronic energy bands in solids: Chapters 1, 2, and 4 to 7;

(ii) atomic physics: Chapters 1 to 6, and 8 to 10;

(iii) elementary particles: Chapters 1 to 6, and 8 to 13.

J.F.Cornwell
St.Andrews
January, 1997

To my wife Elizabeth and my daughters
Rebecca and Jane

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Chapter 1

The Basic Framework

1 The concept of a group

The aim of this chapter is to introduce the idea of a group, to give some physically important examples, and then to indicate immediately how this notion arises naturally in physical problems, and how the related concept of a group representation lies at the heart of the quantum mechanical formulation. With the basic framework established, the next four chapters will explore in more detail the relevant properties of groups and their representations before the application to physical problems is taken up in earnest in Chapter 6.

To mathematicians a group is an object with a very precise meaning. It is a set of elements that must obey four group axioms. On these is based a most elaborate and fascinating theory, not all of which is covered in this book. The development of the theory does not depend on the nature of the elements themselves, but in most physical applications these elements are transformations of one kind or another, which is why T will be used to denote a typical group member.

Definition *Group* $\mathcal{G}$
A set $\mathcal{G}$ of elements is called a "group" if the following four "group axioms" are satisfied:

(a) There exists an operation which associates with every pair of elements T and T' of $\mathcal{G}$ another element T'' of $\mathcal{G}$. This operation is called *multiplication* and is written as $T'' = TT'$, T'' being described as the "product of T with T'".

(b) For any three elements T, T' and T'' of $\mathcal{G}$

$$(TT')T'' = T(T'T''). \tag{1.1}$$

This is known as the "associative law" for group multiplication. (The interpretation of the left-hand side of Equation (1.1) is that the product

TT' is to be evaluated first, and then multiplied by T'' whereas on the right-hand side T is multiplied by the product $T'T''$.)

(c) There exists an *identity element* E which is contained in $\mathcal{G}$ such that

$$TE = ET = T$$

for every element T of $\mathcal{G}$.

(d) For each element T of $\mathcal{G}$ there exists an *inverse element* T^{-1} which is also contained in $\mathcal{G}$ such that

$$TT^{-1} = T^{-1}T = E\,.$$

This definition covers a diverse range of possibilities, as the following examples indicate.

Example I *The multiplicative group of real numbers*
The simplest example (from which the concept of a group was generalized) is the set of all real numbers (excluding zero) with ordinary multiplication as the group multiplication operation. The axioms (a) and (b) are obviously satisfied, the identity is the number 1, and each real number t ($\neq 0$) has its reciprocal $1/t$ as its inverse.

Example II *The additive group of real numbers*
To demonstrate that the group multiplication operation need not have any connection with ordinary multiplication, take $\mathcal{G}$ to be the set of all real numbers with ordinary *addition* as the group multiplication operation. Again axioms (a) and (b) are obviously satisfied, but in this case the identity is 0 (as $a + 0 = 0 + a = a$) and the inverse of a real number a is its negative $-a$ (as $a + (-a) = (-a) + a = 0$).

Example III *A finite matrix group*
Many of the groups appearing in physical problems consist of matrices with matrix multiplication as the group multiplication operation. (A brief account of the terminology and properties of matrices is given in Appendix A.) As an example of such a group let $\mathcal{G}$ be the set of eight matrices

$$\mathbf{M}_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \mathbf{M}_2 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \mathbf{M}_3 = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix},$$

$$\mathbf{M}_4 = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \mathbf{M}_5 = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \quad \mathbf{M}_6 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix},$$

$$\mathbf{M}_7 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \mathbf{M}_8 = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}.$$

By explicit calculation it can be verified that the product of any two members of $\mathcal{G}$ is also contained in $\mathcal{G}$, so that axiom (a) is satisfied. Axiom (b) is

automatically true for matrix multiplication, M_1 is the identity of axiom (c) as it is a unit matrix, and finally axiom (d) is satisfied as

$$\mathbf{M}_1^{-1} = \mathbf{M}_1, \quad \mathbf{M}_2^{-1} = \mathbf{M}_2, \quad \mathbf{M}_3^{-1} = \mathbf{M}_3, \quad \mathbf{M}_4^{-1} = \mathbf{M}_4,$$
$$\mathbf{M}_5^{-1} = \mathbf{M}_6, \quad \mathbf{M}_6^{-1} = \mathbf{M}_5, \quad \mathbf{M}_7^{-1} = \mathbf{M}_7, \quad \mathbf{M}_8^{-1} = \mathbf{M}_8.$$

Example IV *The groups* $\mathrm{U}(N)$ *and* $\mathrm{SU}(N)$

$\mathrm{U}(N)$ for $N \geq 1$ is defined to be the set of all $N \times N$ unitary matrices $\mathbf{u}$ with matrix multiplication as the group multiplication operation. $\mathrm{SU}(N)$ for $N \geq 2$ is defined to be the subset of such matrices $\mathbf{u}$ for which $\det \mathbf{u} = 1$, with the same group multiplication operation. (As noted in Appendix A, if $\mathbf{u}$ is unitary then $\det \mathbf{u} = \exp(i\alpha)$, where α is some real number. The "S" of $\mathrm{SU}(N)$ indicates that $\mathrm{SU}(N)$ is the "special" subset of $\mathrm{U}(N)$ for which this α is zero.)

It is easily established that these sets do form groups. Consider first the set $\mathrm{U}(N)$. As $(\mathbf{u}_1\mathbf{u}_2)^\dagger = \mathbf{u}_2^\dagger \mathbf{u}_1^\dagger$ and $(\mathbf{u}_1\mathbf{u}_2)^{-1} = \mathbf{u}_2^{-1}\mathbf{u}_1^{-1}$, if $\mathbf{u}_1$ and $\mathbf{u}_2$ are both unitary then so is $\mathbf{u}_1\mathbf{u}_2$. Again axiom (b) is automatically valid for matrix multiplication and, as the unit matrix $\mathbf{1}_N$ is a member of $\mathrm{U}(N)$, it provides the identity E of axiom (c). Finally, axiom (d) is satisfied, as if $\mathbf{u}$ is a member of $\mathrm{U}(N)$ then so is $\mathbf{u}^{-1}$.

For $\mathrm{SU}(N)$ the same considerations apply, but in addition if $\mathbf{u}_1$ and $\mathbf{u}_2$ both have determinant 1, Equation (A.4) shows that the same is true of $\mathbf{u}_1\mathbf{u}_2$. Moreover, $\mathbf{1}_N$ is a member of $\mathrm{SU}(N)$, so it is its identity, and $\mathbf{u}^{-1}$ is a member of $\mathrm{SU}(N)$ if that is the case for $\mathbf{u}$.

The set of groups $\mathrm{SU}(N)$ is particularly important in theoretical physics. SU(2) is intimately related to angular momentum and isotopic spin, as will be shown in Chapters 10 and 13, while SU(3) is now famous for its role in the classification of elementary particles, which will also be studied in Chapter 13.

Example V *The groups* $\mathrm{O}(N)$ *and* $\mathrm{SO}(N)$

The set of all $N \times N$ real orthogonal matrices $\mathbf{R}$ (for $N \geq 2$) is denoted almost universally by $\mathrm{O}(N)$, although $\mathrm{O}(N, \mathbb{R})$ would have been preferable as it indicates that only real matrices are included. The subset of such matrices $\mathbf{R}$ with $\det \mathbf{R} = 1$ is denoted by $\mathrm{SO}(N)$. As will be described in Section 2, O(3) and SO(3) are intimately related to rotations in a real three-dimensional Euclidean space, and so occur time and time again in physical applications.

$\mathrm{O}(N)$ and $\mathrm{SO}(N)$ are both groups with matrix multiplication as the group multiplication operation, as they can be regarded as being the subsets of $\mathrm{U}(N)$ and $\mathrm{SU}(N)$ respectively that consist only of real matrices. (All that has to be observed to supplement the arguments given in Example IV is that the product of any two real matrices is real, that $\mathbf{1}_N$ is real, and that the inverse of a real matrix is also real.)

If $T_1T_2 = T_2T_1$ for *every* pair of elements T_1 and T_2 of a group $\mathcal{G}$ (that is, if all T_1 and T_2 of $\mathcal{G}$ *commute*), then $\mathcal{G}$ is said to be "Abelian". It will transpire

	$\mathbf{M}_1$	$\mathbf{M}_2$	$\mathbf{M}_3$	$\mathbf{M}_4$	$\mathbf{M}_5$	$\mathbf{M}_6$	$\mathbf{M}_7$	$\mathbf{M}_8$
$\mathbf{M}_1$	$\mathbf{M}_1$	$\mathbf{M}_2$	$\mathbf{M}_3$	$\mathbf{M}_4$	$\mathbf{M}_5$	$\mathbf{M}_6$	$\mathbf{M}_7$	$\mathbf{M}_8$
$\mathbf{M}_2$	$\mathbf{M}_2$	$\mathbf{M}_1$	$\mathbf{M}_4$	$\mathbf{M}_3$	$\mathbf{M}_8$	$\mathbf{M}_7$	$\mathbf{M}_6$	$\mathbf{M}_5$
$\mathbf{M}_3$	$\mathbf{M}_3$	$\mathbf{M}_4$	$\mathbf{M}_1$	$\mathbf{M}_2$	$\mathbf{M}_6$	$\mathbf{M}_5$	$\mathbf{M}_8$	$\mathbf{M}_7$
$\mathbf{M}_4$	$\mathbf{M}_4$	$\mathbf{M}_3$	$\mathbf{M}_2$	$\mathbf{M}_1$	$\mathbf{M}_7$	$\mathbf{M}_8$	$\mathbf{M}_5$	$\mathbf{M}_6$
$\mathbf{M}_5$	$\mathbf{M}_5$	$\mathbf{M}_7$	$\mathbf{M}_6$	$\mathbf{M}_8$	$\mathbf{M}_3$	$\mathbf{M}_1$	$\mathbf{M}_4$	$\mathbf{M}_2$
$\mathbf{M}_6$	$\mathbf{M}_6$	$\mathbf{M}_8$	$\mathbf{M}_5$	$\mathbf{M}_7$	$\mathbf{M}_1$	$\mathbf{M}_3$	$\mathbf{M}_2$	$\mathbf{M}_4$
$\mathbf{M}_7$	$\mathbf{M}_7$	$\mathbf{M}_5$	$\mathbf{M}_8$	$\mathbf{M}_6$	$\mathbf{M}_2$	$\mathbf{M}_4$	$\mathbf{M}_1$	$\mathbf{M}_3$
$\mathbf{M}_8$	$\mathbf{M}_8$	$\mathbf{M}_6$	$\mathbf{M}_7$	$\mathbf{M}_5$	$\mathbf{M}_4$	$\mathbf{M}_2$	$\mathbf{M}_3$	$\mathbf{M}_1$

Table 1.1: Multiplication table for the group of Example III.

that such groups have relatively straightforward properties. However, many of the groups having physical applications are non-Abelian. Of the cases considered above the only Abelian groups are those of Examples I and II and the groups U(1) and SO(2) of Examples IV and V. (One of the non-commuting pairs of products of Example III which makes that group non-Abelian is $\mathbf{M}_5\mathbf{M}_7 = \mathbf{M}_4$, $\mathbf{M}_7\mathbf{M}_5 = \mathbf{M}_2$.)

The "order" of $\mathcal{G}$ is defined to be the number of elements in $\mathcal{G}$, which may be finite, countably infinite, or even non-countably infinite. A group with finite order is called a "finite group". The vast majority of groups that arise in physical situations are either finite groups or are "Lie groups", which are a special type of group of non-countably infinite order whose precise definition will be given in Chapter 3, Section 1. Example III is a finite group of order 8, whereas Examples I, II, IV and V are all Lie groups.

For a finite group the product of every element with every other element is conveniently displayed in a multiplication table, from which all information on the structure of the group can subsequently be deduced. The multiplication table of Example III is given in Table 1.1. (By convention the order of elements in a product is such that the element in the left-hand column precedes the element in the top row, so for example $\mathbf{M}_5\mathbf{M}_8 = \mathbf{M}_2$.) For groups of infinite order the construction of a multiplication table is clearly completely impractical, but fortunately for a Lie group the structure of the group is very largely determined by another finite set of relations, namely the commutation relations between the basis elements of the corresponding real Lie algebra, as will be explained in detail in Chapter 8.

2 Groups of coordinate transformations

To proceed beyond an intuitive picture of the effect of symmetry operations, it is necessary to specify the operations in a precise algebraic form so that the results of successive operations can be easily deduced. Attention will be confined here to transformations in a real three-dimensional Euclidean space $\mathbb{R}^3$, as most applications in atomic, molecular and solid state physics involve only transformations of this type.

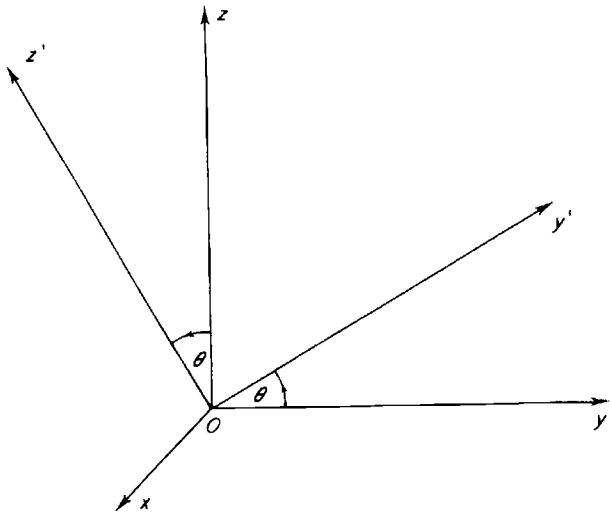

Figure 1.1: Effect of a rotation through an angle θ in the right-hand screw sense about Ox.

(a) Rotations

Let Ox, Oy, Oz be three mutually orthogonal Cartesian axes and let Ox', Oy', Oz' be another set of mutually orthogonal Cartesian axes with the same origin O that is obtained from the first set by a rotation T about a specified axis through O. Let (x, y, z) and (x', y', z') be the coordinates of a fixed point P in the space with respect to these two sets of axes. Then there exists a real orthogonal 3×3 matrix $\mathbf{R}(T)$ which depends on the rotation T, but which is independent of the position of P, such that

$$\mathbf{r}' = \mathbf{R}(T)\mathbf{r}, \tag{1.2}$$

where

$$\mathbf{r}' = \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} \text{ and } \mathbf{r} = \begin{bmatrix} x \\ y \\ z \end{bmatrix}.$$

(Hereafter position vectors will always be considered as 3×1 column matrices in matrix expressions unless otherwise indicated, although for typographical reasons they will often be displayed in the text as 1×3 row matrices.) For example, if T is a rotation through an angle θ in the right-hand screw sense about the axis Ox, then, as indicated in Figures 1.1 and 1.2,

$$\begin{aligned} x' &= x, \\ y' &= y\cos\theta + z\sin\theta, \\ z' &= -y\sin\theta + z\cos\theta, \end{aligned}$$

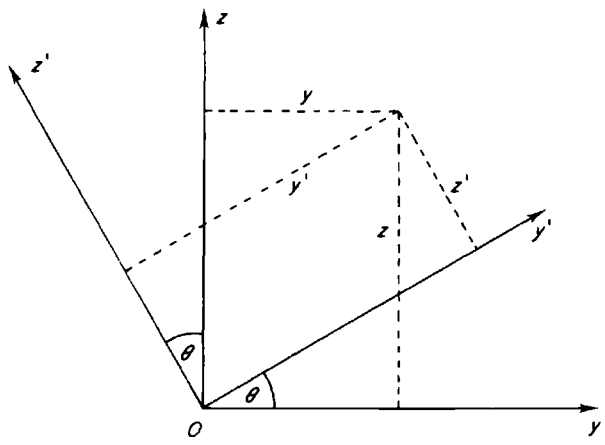

Figure 1.2: The plane containing the axes Oy, Oz, Oy' and Oz' corresponding to the rotation of Figure 1.1.

so that

$$\mathbf{R}(T) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{bmatrix}. \tag{1.3}$$

The matrix $\mathbf{R}(T)$ obeys the orthogonality condition $\widetilde{\mathbf{R}}(T) = \mathbf{R}(T)^{-1}$ because rotations leave invariant the length of every position vector and the angle between every pair of position vectors, that is, they leave invariant the scalar product $\mathbf{r}_1.\mathbf{r}_2$ of any two position vectors. (Indeed the name "orthogonal" stems from the involvement of such matrices in the transformations being considered here between sets of orthogonal axes.) The proof that $\mathbf{R}(T)$ is orthogonal depends on the fact that $\mathbf{r}_1.\mathbf{r}_2$ can be expressed in matrix form as $\widetilde{\mathbf{r}}_1\mathbf{r}_2$. Then, if $\mathbf{r}'_1 = \mathbf{R}(T)\mathbf{r}_1$ and $\mathbf{r}'_2 = \mathbf{R}(T)\mathbf{r}_2$, it follows that $\mathbf{r}'_1.\mathbf{r}_2 = \widetilde{\mathbf{r}}'_1\mathbf{r}'_2 = \widetilde{\mathbf{r}}_1\widetilde{\mathbf{R}}(T)\mathbf{R}(T)\mathbf{r}_2$, which is equal to $\widetilde{\mathbf{r}}_1\mathbf{r}_2$ for all $\mathbf{r}_1$ and $\mathbf{r}_2$ if and only if $\widetilde{\mathbf{R}}(T)\mathbf{R}(T) = \mathbf{1}$.

As noted in Appendix A, the orthogonality condition implies that $\det \mathbf{R}(T)$ can take only the values $+1$ or -1. If $\det \mathbf{R}(T) = +1$ the rotation is said to be "proper"; otherwise it is said to be "improper". The only rotations which can be applied to a rigid body are proper rotations. The transformation of Equation (1.3) gives an example.

The simplest example of an improper rotation is the spatial inversion operation I for which $\mathbf{r}' = -\mathbf{r}$, so that

$$\mathbf{R}(I) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}.$$

Another important example is the operation of reflection in a plane. For instance, for reflection in the plane Oyz, for which $x' = -x, y' = y, z' = z$,

the transformation matrix is

$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

The "product" T_1T_2 of two rotations T_1 and T_2 may be *defined* to be the rotation whose transformation matrix is given by

$$\mathbf{R}(T_1T_2) = \mathbf{R}(T_1)\mathbf{R}(T_2). \tag{1.4}$$

(The validity of this definition is assured by the fact that the product of any two real orthogonal matrices is itself real and orthogonal.) In general $\mathbf{R}(T_1)\mathbf{R}(T_2) \neq \mathbf{R}(T_2)\mathbf{R}(T_1)$, in which case $T_1T_2 \neq T_2T_1$. If $\mathbf{r}' = \mathbf{R}(T_2)\mathbf{r}$ and $\mathbf{r}'' = \mathbf{R}(T_1)\mathbf{r}'$, then Equation (1.4) implies that $\mathbf{r}'' = \mathbf{R}(T_1T_2)\mathbf{r}$, so the interpretation of Equation (1.4) is that operation T_2 takes place *before* T_1. This is an example of the general convention (which will be applied throughout this book) that in any product of operators the operator on the right acts first.

With this definition (Equation (1.4)) every improper rotation can be considered to be the product of the spatial inversion operator I with a proper rotation. For example, for the reflection in the Oyz plane

$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix},$$

and, as the second matrix on the right-hand side is the transformation of Equation (1.3) with $\theta = \pi$, it corresponds to a rotation through π about Ox.

If a set of matrices $\mathbf{R}(T)$ forms a group, then the corresponding set of rotations T also forms a group in which Equation (1.4) defines the group multiplication operator and for which the inverse T^{-1} of T is given by $\mathbf{R}(T^{-1}) = \mathbf{R}(T)^{-1}$. As these two groups have the same structure, they are said to be "isomorphic" (a concept which will be examined in more detail in Chapter 2, Section 6).

Example I *The group of all rotations*
The set of all rotations, both proper and improper, forms a Lie group that is isomorphic to the group O(3) that was introduced in Example V of Section 1.

Example II *The group of all proper rotations*
The set of all proper rotations forms a Lie group that is isomorphic to the group SO(3).

Example III *The crystallographic point group D_4*
A group of rotations that leave invariant a crystal lattice is called a "crystallographic point group", the "point" indicating that one point, the origin O, is left unmoved by the operations of the group. There are only 32 such

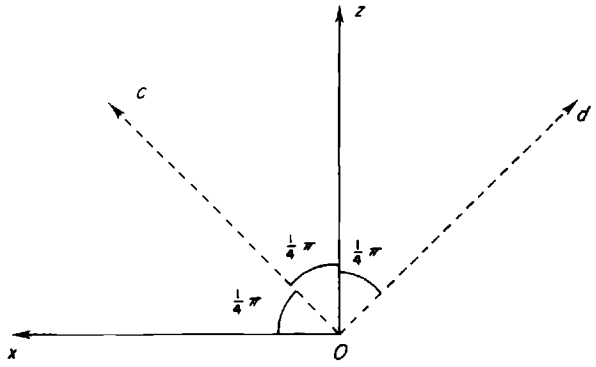

Figure 1.3: The rotation axes Ox, Oz, Oc and Od of the crystallographic point group D_4.

groups, all of which are finite. A complete description is given in Appendix C. The only possible angles of rotation are $2\pi/n$, where $n = 2$, 3, 4, or 6. (This restriction on the value of n is a consequence of the translational symmetry of a perfect crystal (cf. Chapter 7, Section 6). For a "quasicrystal", which has no such translational symmetry, this restriction no longer applies, and so it is possible to have other values of n as well, including, in particular, the value $n = 5$.) It is convenient to denote a proper rotation through $2\pi/n$ about an axis Oj by C_{nj}. The identity transformation may be denoted by E, so that $\mathbf{R}(E) = \mathbf{1}$, and improper rotations can be written in the form IC_{nj}. As an example, consider the crystallographic point group D_4, the notation being that of Schönfliess (1923). D_4 consists of the eight rotations:

E: the identity;

C_{2x}, C_{2y}, C_{2z}: proper rotations through π about Ox, Oy, Oz respectively;

C_{4y}, C_{4y}^{-1}: proper rotations through $\pi/2$ about Oy in the right-hand and left-hand screw senses respectively;

C_{2c}, C_{2d}: proper rotations through π about Oc and Od respectively.

Here Ox, Oy, Oz are mutually orthogonal Cartesian axes, and Oc, Od are mutually orthogonal axes in the plane Oxz with Oc making an angle of $\pi/4$ with both Ox and Oz, as indicated in Figure 1.3. The transformation matrices are

$$\mathbf{R}(E) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \mathbf{R}(C_{2x}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix},$$

$$\mathbf{R}(C_{2y}) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \quad \mathbf{R}(C_{2z}) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

$$\mathbf{R}(C_{4y}) = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad \mathbf{R}(C_{4y}^{-1}) = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix},$$

$$\mathbf{R}(C_{2c}) = \begin{bmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad \mathbf{R}(C_{2d}) = \begin{bmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{bmatrix}.$$

	E	C_{2x}	C_{2y}	C_{2z}	C_{4y}	C_{4y}^{-1}	C_{2c}	C_{2d}
E	E	C_{2x}	C_{2y}	C_{2z}	C_{4y}	C_{4y}^{-1}	C_{2c}	C_{2d}
C_{2x}	C_{2x}	E	C_{2z}	C_{2y}	C_{2d}	C_{2c}	C_{4y}^{-1}	C_{4y}
C_{2y}	C_{2y}	C_{2z}	E	C_{2x}	C_{4y}^{-1}	C_{4y}	C_{2d}	C_{2c}
C_{2z}	C_{2z}	C_{2y}	C_{2x}	E	C_{2c}	C_{2d}	C_{4y}	C_{4y}^{-1}
C_{4y}	C_{4y}	C_{2c}	C_{4y}^{-1}	C_{2d}	C_{2y}	E	C_{2z}	C_{2x}
C_{4y}^{-1}	C_{4y}^{-1}	C_{2d}	C_{4y}	C_{2c}	E	C_{2y}	C_{2x}	C_{2z}
C_{2c}	C_{2c}	C_{4y}	C_{2d}	C_{4y}^{-1}	C_{2x}	C_{2z}	E	C_{2y}
C_{2d}	C_{2d}	C_{4y}^{-1}	C_{2c}	C_{4y}	C_{2z}	C_{2x}	C_{2y}	E

Table 1.2: Multiplication table for the crystallographic point group D_4.

The multiplication table is given in Table 1.2. This example will be used to illustrate a number of concepts in Chapters 2, 4, 5 and 6.

(b) Translations

Suppose now that Ox, Oy, Oz is a set of mutually orthogonal Cartesian axes and $O'x', O'y', O'z'$ is another set, obtained by first rotating the original set about some axis through O by a rotation whose transformation matrix is $\mathbf{R}(T)$, and then translating O to O' along a vector $-\mathbf{t}(T)$ without further rotation. (In $\mathbb{R}^3$ any two sets of Cartesian axes can be related in this way.) Then Equation (1.2) generalizes to

$$\mathbf{r}' = \mathbf{R}(T)\mathbf{r} + \mathbf{t}(T). \tag{1.5}$$

It is useful to regard the rotation and translation as being two parts of a *single* coordinate transformation T, and so it is convenient to rewrite Equation (1.5) as

$$\mathbf{r}' = \{\mathbf{R}(T)|\mathbf{t}(T)\}\mathbf{r},$$

thereby defining the composite operator $\{\mathbf{R}(T)|\mathbf{t}(T)\}$. Indeed, in the non-symmorphic space groups (see Chapter 7, Section 6), there exist symmetry operations in which the combined rotation and translation leave the crystal lattice invariant without this being true for the rotational and translational parts separately.

The generalization of Equation (1.4) can be deduced by considering the two successive transformations $\mathbf{r}' = \{\mathbf{R}(T_2)|\mathbf{t}(T_2)\}\mathbf{r} \equiv \mathbf{R}(T_2)\mathbf{r} + \mathbf{t}(T_2)$ and $\mathbf{r}'' = \{\mathbf{R}(T_1)|\mathbf{t}(T_1)\}\mathbf{r}' \equiv \mathbf{R}(T_1)\mathbf{r}' + \mathbf{t}(T_1)$, which give

$$\mathbf{r}'' = \mathbf{R}(T_1)\mathbf{R}(T_2)\mathbf{r} + [\mathbf{R}(T_1)\mathbf{t}(T_2) + \mathbf{t}(T_1)]. \tag{1.6}$$

Thus the natural choice of the definition of the "product" T_1T_2 of two general symmetry operations T_1 and T_2 is

$$\{\mathbf{R}(T_1)|\mathbf{t}(T_1)\} = \{\mathbf{R}(T_1)\mathbf{R}(T_2)\,|\,\mathbf{R}(T_1)\mathbf{t}(T_2) + \mathbf{t}(T_1)\}. \tag{1.7}$$

This product always satisfies the group associative law of Equation (1.1).

As Equation (1.5) can be inverted to give

$$\mathbf{r} = \mathbf{R}(T)^{-1}\mathbf{r}' - \mathbf{R}(T)^{-1}\mathbf{t}(T),$$

the inverse of $\{\mathbf{R}(T)|\mathbf{t}(T)\}$ may be defined by

$$\{\mathbf{R}(T)|\mathbf{t}(T)\}^{-1} = \{\mathbf{R}(T)^{-1}\,|\,-\mathbf{R}(T)^{-1}\mathbf{t}(T)\}. \tag{1.8}$$

It is easily verified that

$$\{\mathbf{R}(T_1T_2)|\mathbf{t}(T_1T_2)\}^{-1} = \{\mathbf{R}(T_2)|\mathbf{t}(T_2)\}^{-1}\{\mathbf{R}(T_1)|\mathbf{t}(T_1)\}^{-1}, \tag{1.9}$$

the order of factors being reversed on the right-hand side.

It is sometimes convenient to refer to transformations for which $\mathbf{t}(T) = \mathbf{0}$ as "pure rotations" and those for which $\mathbf{R}(T) = \mathbf{1}$ as "pure translations".

3 The group of the Schrödinger equation

(a) The Hamiltonian operator

The Hamiltonian operator H of a physical system plays two major roles in quantum mechanics (Schiff 1968). Firstly, its eigenvalues ϵ, as given by the time-independent Schrödinger equation

$$H\phi = \epsilon\phi,$$

are the only allowed values of the energy of the system. Secondly, the time development of the system is determined by a wave function $\psi(t)$ which satisfies the time-dependent Schrödinger equation

$$H\psi = i\hbar\partial\psi/\partial t.$$

Not surprisingly, a considerable amount can be learnt about the system by simply examining the set of transformations which leave the Hamiltonian invariant. Indeed the main function of group theory, as it is applied in physical problems, is to systematically extract as much information as possible from this set of transformations.

In order to present the essential features as clearly as possible, it will be assumed in the first instance that the problem involves solving a "single-particle" Schrödinger equation. That is, it will be supposed that either the system contains only one particle, or, if there is more than one particle involved, then they do not interact or their inter-particle interactions have been

treated in a Hartree-Fock or similar approximation in such a way that each particle experiences only the average field of all of the others. Moreover, it will be assumed that H contains no spin-dependent terms, so that the significant part of every wave function is a scalar function. For example, for an electron in this situation, each wave function can be taken to be the product of an "orbital" function, which is a scalar, with one of two possible spin functions, so that the only effect of the electron's spin is to double the "orbital" degeneracy of each energy eigenvalue. (A development of a theory of spinors along similar lines that enables spin-dependent Hamiltonians to be studied is given, for example, in Chapter 6, Section 4, of Cornwell (1984).)

With these assumptions a typical Hamiltonian operator for a particle of mass μ has the form

$$H(\mathbf{r}) = -\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(\mathbf{r}), \tag{1.10}$$

where $V(\mathbf{r})$ is the potential field experienced by the particle. For example, for the electron of a hydrogen atom whose nucleus is located at O,

$$H(\mathbf{r}) = -\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) - e^2/\{x^2 + y^2 + z^2\}^{1/2}. \tag{1.11}$$

In Equations (1.10) and (1.11) the Hamiltonian is written as $H(\mathbf{r})$ to emphasize its dependence on the particular coordinate system $Oxyz$.

(b) The invariance of the Hamiltonian operator

Let $H(\{\mathbf{R}(T)|\mathbf{t}(T)\}\mathbf{r})$ be the operator that is obtained from $H(\mathbf{r})$ by substituting the components of $\mathbf{r}' = \{\mathbf{R}(T)|\mathbf{t}(T)\}\mathbf{r}$ in place of the corresponding components of $\mathbf{r}$. For example, if $H(\mathbf{r})$ is given by Equation (1.11), then

$$H(\{\mathbf{R}(T)|\mathbf{t}(T)\}\mathbf{r}) = -\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial x'^2} + \frac{\partial^2}{\partial y'^2} + \frac{\partial^2}{\partial z'^2}\right) - e^2/\{x'^2 + y'^2 + z'^2\}^{1/2}. \tag{1.12}$$

$H(\{\mathbf{R}(T)|\mathbf{t}(T)\}\mathbf{r})$ can then be rewritten so that it depends *explicitly* on $\mathbf{r}$. For example, in Equation (1.12), if T is a pure translation $x' = x + t_1, y' = y + t_2, z' = z + t_3$, then

$$\begin{aligned} H(\{\mathbf{R}(T)|\mathbf{t}(T)\}\mathbf{r}) \quad = \quad & -\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) \\ & -e^2/\{(x + t_1)^2 + (y + t_2)^2 + (z + t_3)^2\}^{1/2}. \end{aligned}$$

so that

$$H(\{\mathbf{R}(T)|\mathbf{t}(T)\}\mathbf{r}) \neq H(\mathbf{r}),$$

whereas if T is a pure rotation about O, then a short algebraic calculation gives

$$H(\{\mathbf{R}(T)|\mathbf{t}(T)\}\mathbf{r}) = -\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) - e^2/\{x^2 + y^2 + z^2\}^{1/2},$$

and hence in this case

$$H(\{\mathbf{R}(T)|\mathbf{t}(T)\}\mathbf{r}) = H(\mathbf{r}).$$

A coordinate transformation T for which

$$H(\{\mathbf{R}(T)|\mathbf{t}(T)\}\mathbf{r}) = H(\mathbf{r}) \tag{1.13}$$

is said to leave the Hamiltonian "invariant". For the hydrogen atom the above analysis merely explicitly demonstrates the intuitively obvious fact that the system is invariant under pure rotations but not under pure translations.

The following key theorem shows how and why group theory plays such a significant part in quantum mechanics.

Theorem I The set of coordinate transformations that leave the Hamiltonian invariant form a group. This group is usually called "the group of the Schrödinger equation", but is sometimes referred to as "the invariance group of the Hamiltonian operator".

Proof It has only to be verified that the four group axioms are satisfied. Firstly, if the Hamiltonian is invariant under two separate coordinate transformations T_1 and T_2, then it is invariant under their product T_1T_2. (Invariance under T_1 implies that $H(\mathbf{r}'') = H(\mathbf{r}')$, where $\mathbf{r}'' = \{\mathbf{R}(T_1)|\mathbf{t}(T_1)\}\mathbf{r}'$, and invariance under T_2 implies that $H(\mathbf{r}') = H(\mathbf{r})$, where $\mathbf{r}' = \{\mathbf{R}(T_2)|\mathbf{t}(T_2)\}\mathbf{r}$, so that $H(\mathbf{r}'') = H(\mathbf{r})$, where, by Equation (1.7), $\mathbf{r}'' = \{\mathbf{R}(T_1T_2)|\mathbf{t}(T_1T_2)\}\mathbf{r}$). Secondly, as noted in Section 2(b), the associative law is valid for all coordinate transformations. Thirdly, the identity transformation obviously leaves the Hamiltonian invariant, and finally, as Equation (1.13) can be rewritten as $H(\mathbf{r}') = H(\{\mathbf{R}(T)|\mathbf{t}(T)\}^{-1}\mathbf{r}')$, where $\mathbf{r}' = \{\mathbf{R}(T)|\mathbf{t}(T)\}\mathbf{r}$, if T leaves the Hamiltonian invariant then so does T^{-1}.

For the case of the hydrogen atom, or any other spherically symmetric system in which $V(\mathbf{r})$ is a function of $|\mathbf{r}|$ alone, the group of the Schrödinger equation is the group of all pure rotations in $\mathbb{R}^3$.

(c) The scalar transformation operators $P(T)$

A "scalar field" is defined to be a quantity that takes a value at each point in the space $\mathbb{R}^3$ (in general taking different values at different points), the value at a point being independent of the choice of coordinate system that is used to designate the point. One of the simplest examples to visualize is the density of particles. The concept is relevant to the present consideration because the "orbital" part of an electron's wave function is a scalar field.

Suppose that the scalar field is specified by a function $\psi(\mathbf{r})$ when the coordinates of points of $\mathbb{R}^3$ are defined by a coordinate system Ox, Oy, Oz, and that the same scalar field is specified by a function $\psi'(\mathbf{r}')$ when another coordinate system $O'x', O'y', O'z'$ is used instead. If $\mathbf{r}$ and $\mathbf{r}'$ are the position

vectors of the same point referred to the two coordinate systems, then the definition of the scalar field implies that

$$\psi'(\mathbf{r}') = \psi(\mathbf{r}). \tag{1.14}$$

Now suppose that $O'x', O'y', O'z'$ are obtained from Ox, Oy, Oz by a coordinate transformation T, so that $\mathbf{r}' = \{\mathbf{R}(T)|\mathbf{t}(T)\}\mathbf{r}$.

Then Equation (1.14) can be written as

$$\psi'(\mathbf{r}') = \psi(\{\mathbf{R}(T)|\mathbf{t}(T)\}^{-1}\mathbf{r}'), \tag{1.15}$$

which provides a concrete prescription for determining the function ψ' from the function ψ, namely that $\psi'(\mathbf{r}')$ is the function obtained by replacing each component of $\mathbf{r}$ in $\psi(\mathbf{r})$ by the corresponding component of $\{\mathbf{R}(T)|\mathbf{t}(T)\}^{-1}\mathbf{r}'$. For example, if $\psi(\mathbf{r}) = x^2y^3$ and T is the pure rotation of Equation (1.3), as

$$\begin{aligned} \{\mathbf{R}(T)|\mathbf{t}(T)\}^{-1}\mathbf{r}' &= \mathbf{R}(T)^{-1}\mathbf{r}' = \widetilde{\mathbf{R}}(T)\mathbf{r}' \\ &= (x', y'\cos\theta - z'\sin\theta, y'\sin\theta + z'\cos\theta), \end{aligned}$$

then

$$\psi'(\mathbf{r}') = x'^2(y'\cos\theta - z'\sin\theta)^3.$$

It is very convenient in the following analysis to replace the argument $\mathbf{r}'$ of ψ' by $\mathbf{r}$ (without changing the functional form of ψ'). Thus in the above example

$$\psi'(\mathbf{r}) = x(y\cos\theta - z\sin\theta)^3,$$

and Equation (1.15) can be rewritten as

$$\psi'(\mathbf{r}) = \psi(\{\mathbf{R}(T)|\mathbf{t}(T)\}^{-1}\mathbf{r}). \tag{1.16}$$

As $\psi'(\mathbf{r})$ is uniquely determined from $\psi(\mathbf{r})$ for the coordinate transformation T, ψ' can be regarded as being obtained from ψ by the action of an *operator* $P(T)$, which is therefore *defined* by $\psi' = P(T)\psi$, or, equivalently, from Equation (1.16) by

$$(P(T)\psi)(\mathbf{r}) = \psi(\{\mathbf{R}(T)|\mathbf{t}(T)\}^{-1}\mathbf{r}).$$

The typography can be simplified without causing confusion by removing one of the sets of brackets on the left-hand side, giving

$$P(T)\psi(\mathbf{r}) = \psi(\{\mathbf{R}(T)|\mathbf{t}(T)\}^{-1}\mathbf{r}). \tag{1.17}$$

These scalar transformation operators perform a particularly important role in the application of group theory to quantum mechanics. Their properties will now be established.

Clearly $P(T_1) = P(T_2)$ only if $T_1 = T_2$. (Here $P(T_1) = P(T_2)$ means that $P(T_1)\psi(\mathbf{r}) = P(T_2)\psi(\mathbf{r})$ for *every* function $\psi(\mathbf{r})$.) Moreover, each operator $P(T)$ is *linear*, that is

$$P(T)\{a\phi(\mathbf{r}) + b\psi(\mathbf{r})\} = aP(T)\phi(\mathbf{r}) + bP(T)\psi(\mathbf{r}) \tag{1.18}$$

for any two functions $\phi(\mathbf{r})$ and $\psi(\mathbf{r})$ and any two complex numbers a and b, as can be verified directly from Equation (1.17); (see Appendix B, Section 4). The other major properties of the operators $P(T)$ are most succinctly stated in the following four theorems.

Theorem II Each operator $P(T)$ is a *unitary* operator in the Hilbert space L^2 with inner product (ϕ, ψ) defined by

$$(\phi, \psi) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \phi^*(\mathbf{r})\psi(\mathbf{r})\, dx\, dy\, dz, \tag{1.19}$$

where the integral is over the whole of the space $\mathbb{R}^3$, that is,

$$(P(T)\phi, P(T)\psi) = (\phi, \psi) \tag{1.20}$$

for any two functions ϕ and ψ of L^2; (see Appendix B, Sections 3 and 4).

Proof With $\mathbf{r}''$ defined by $\mathbf{r}'' = \{\mathbf{R}(T)|\mathbf{t}(T)\}^{-1}\mathbf{r}$, from Equations (1.17) and (1.19)

$$(P(T)\phi, P(T)\psi) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \phi^*(\mathbf{r}'')\psi(\mathbf{r}'')\, dx\, dy\, dz. \tag{1.21}$$

However, $dx\, dy\, dz = J\, dx''\, dy''\, dz''$, where the Jacobian J is defined by

$$J = \det \begin{bmatrix} \partial x/\partial x'' & \partial x/\partial y'' & \partial x/\partial z'' \\ \partial y/\partial x'' & \partial y/\partial y'' & \partial y/\partial z'' \\ \partial z/\partial x'' & \partial z/\partial y'' & \partial z/\partial z'' \end{bmatrix}$$

As $\mathbf{r} = \mathbf{R}(T)\mathbf{r}'' + \mathbf{t}(T)$, it follows that $\partial x/\partial x'' = R(T)_{11}, \partial x/\partial y'' = R(T)_{12}$ etc., so that $J = \det \mathbf{R}(T) = \pm 1$. In converting the right-hand side of Equation (1.21) to a triple integral with respect to x'', y'', z'', there appears an odd number of interchanges of upper and lower limits for an improper rotation, whereas for a proper rotation there is an even number of such interchanges. (For example, for spatial inversion I, $x'' = -x, y'' = -y, z'' = -z$, so the upper and lower limits are interchanged three times, while for a rotation through π about Oz the limits are interchanged twice.) Thus in all cases Equation (1.21) can be written as

$$(P(T)\phi, P(T)\psi) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \phi^*(\mathbf{r}'')\psi(\mathbf{r}'')\, dx''\, dy''\, dz'',$$

from which Equation (1.20) follows immediately.

Theorem III For any two coordinate transformations T_1 and T_2,

$$P(T_1T_2) = P(T_1)P(T_2). \tag{1.22}$$

Proof It is required to show that for *any* function $\psi(\mathbf{r})$, $P(T_1T_2)\psi(\mathbf{r}) = P(T_1)P(T_2)\psi(\mathbf{r})$, where in the right-hand side $P(T_2)$ acts first on $\psi(\mathbf{r})$ and

$P(T_1)$ acts on the resulting expression. Let $\phi(\mathbf{r}) = P(T_2)\psi(\mathbf{r})$, so that $\phi(\mathbf{r}) = \psi(\{\mathbf{R}(T_2)|\mathbf{t}(T_2)\}^{-1}\mathbf{r})$. Then

$$P(T_1)\phi(\mathbf{r}) = \phi(\{\mathbf{R}(T_1)|\mathbf{t}(T_1)\}^{-1}\mathbf{r}) = \psi(\{\mathbf{R}(T_2)|\mathbf{t}(T_2)\}^{-1}\{\mathbf{R}(T_1)|\mathbf{t}(T_1)\}^{-1}\mathbf{r}),$$

the last equality being a consequence of the fact that $\phi(\{\mathbf{R}(T_1)|\mathbf{t}(T_1)\}^{-1}\mathbf{r})$ is by definition the function obtained from $\phi(\mathbf{r})$ by simply replacing the components of $\mathbf{r}$ by the components of $\{\mathbf{R}(T_1)|\mathbf{t}(T_1)\}^{-1}\mathbf{r}$. Thus, on using Equation (1.9),

$$P(T_1)P(T_2)\psi(\mathbf{r}) = \psi(\{\mathbf{R}(T_1T_2)|\mathbf{t}(T_1T_2)\}^{-1}\mathbf{r}) = P(T_1T_2)\psi(\mathbf{r}).$$

Theorem IV The set of operators $P(T)$ that correspond to the coordinate transformations T of the group of the Schrödinger equation forms a group that is isomorphic to the group of the Schrödinger equation.

Proof The product $P(T_1)P(T_2)$, as defined in the proof of the previous theorem, may be taken to specify the group multiplication operation, so that the associative law of axiom (b) is satisfied. The previous theorem then implies that group axiom (a) is fulfilled, and with $P(E)$ being the identity operator it also implies that the inverse operator $P(T)^{-1}$ may be defined by $P(T)^{-1} = P(T^{-1})$. Finally, it also indicates that the two groups are isomorphic.

Theorem V For every coordinate transformation T of the group of the Schrödinger equation $\mathcal{G}$

$$P(T)H(\mathbf{r}) = H(\mathbf{r})P(T). \tag{1.23}$$

Proof It has to be established that for any $\psi(\mathbf{r})$ and any T of $\mathcal{G}$

$$P(T)\{H(\mathbf{r})\psi(\mathbf{r})\} = H(\mathbf{r})\{P(T)\psi(\mathbf{r})\}. \tag{1.24}$$

Let $\phi(\mathbf{r}) = H(\mathbf{r})\psi(\mathbf{r})$. Then, by Equation (1.17),

$$\begin{aligned} P(T)\phi(\mathbf{r}) &= \phi(\{\mathbf{R}(T)|\mathbf{t}(T)\}^{-1}\mathbf{r}) \\ &= H(\{\mathbf{R}(T)|\mathbf{t}(T)\}^{-1}\mathbf{r})\psi(\{\mathbf{R}(T)|\mathbf{t}(T)\}^{-1}\mathbf{r}) \\ &= H(\{\mathbf{R}(T)|\mathbf{t}(T)\}^{-1}\mathbf{r})\{P(T)\psi(\mathbf{r})\}, \end{aligned}$$

from which Equation (1.24) follows by Equation (1.13).

4 The role of matrix representations

Having shown how groups arise naturally in quantum mechanics, in this preliminary survey it remains only to introduce the concept of a group representation and to demonstrate that it too has a fundamental role to play.

Definition *Representation of a group*
If each element T of a group $\mathcal{G}$ can be assigned a non-singular $d \times d$ matrix $\mathbf{\Gamma}(T)$ contained in a group of matrices having matrix multiplication as its group multiplication operation in such a way that

$$\mathbf{\Gamma}(T_1 T_2) = \mathbf{\Gamma}(T_1)\mathbf{\Gamma}(T_2) \tag{1.25}$$

for every pair of elements T_1 and T_2 of $\mathcal{G}$, then this set of matrices is said to provide a d-dimensional "representation" $\mathbf{\Gamma}$ of $\mathcal{G}$.

Example I *A representation of the crystallographic point group D_4*
The group D_4 introduced in Example III of Section2 has the following two-dimensional representation:

$$\begin{array}{llll} \mathbf{\Gamma}(E) = \mathbf{M}_1, & \mathbf{\Gamma}(C_{2x}) = \mathbf{M}_2, & \mathbf{\Gamma}(C_{2y}) = \mathbf{M}_3, & \mathbf{\Gamma}(C_{2z}) = \mathbf{M}_4, \\ \mathbf{\Gamma}(C_{4y}) = \mathbf{M}_5, & \mathbf{\Gamma}(C_{4y}^{-1}) = \mathbf{M}_6, & \mathbf{\Gamma}(C_{2c}) = \mathbf{M}_7, & \mathbf{\Gamma}(C_{2d}) = \mathbf{M}_8, \end{array}$$

where $\mathbf{M}_1, \mathbf{M}_2, \ldots$ are the 2×2 matrices defined in Example III of Section 1. That Equation (1.25) is satisfied can be verified simply by comparing Tables 1.1 and 1.2.

It will be shown in Chapter 4 that every group has an infinite number of different representations, but they are derivable from a smaller number of basic representations, the so-called "irreducible representations". A finite group has only a finite number of such irreducible representations that are essentially different.

The representations of the group of the Schrödinger equation are of particular interest. The intimate connection between them and the eigenfunctions of the time-independent Schrödinger equation is provided by the notion of "basis functions" of the representations.

Definition *Basis functions of a group of coordinate transformations $\mathcal{G}$*
A set of d linearly independent functions $\psi_1(\mathbf{r}), \psi_2(\mathbf{r}), \ldots, \psi_d(\mathbf{r})$ forms a basis for a d-dimensional representation $\mathbf{\Gamma}$ of $\mathcal{G}$ if, for every coordinate transformation T of $\mathcal{G}$,

$$P(T)\psi_n(\mathbf{r}) = \sum_{m=1}^{d} \Gamma(T)_{mn}\psi_m(\mathbf{r}), \quad n = 1, 2, \ldots, d. \tag{1.26}$$

The function $\psi_n(\mathbf{r})$ is then said to "transform as the nth row" of the representation $\mathbf{\Gamma}$.

The definition implies that not only is each function $P(T)\psi_n(\mathbf{r})$ required to be a linear combination of $\psi_1(\mathbf{r}), \psi_2(\mathbf{r}), \ldots, \psi_d(\mathbf{r})$, but the coefficients are required to be equal to specified matrix elements of $\mathbf{\Gamma}(T)$. The rather unusual ordering of row and column indices on the right-hand side of Equation (1.26)

ensures the consistency of the definition for every product T_1T_2, for, according to Equations (1.18), (1.22), (1.25), and (1.26),

$$\begin{aligned} P(T_1T_2)\psi_n(\mathbf{r}) &= P(T_1)P(T_2)\psi_n(\mathbf{r}) \\ &= P(T_1)\{\sum_{m=1}^{d}\Gamma(T_2)_{mn}\psi_m(\mathbf{r})\} \\ &= \sum_{m=1}^{d}\Gamma(T_2)_{mn}P(T_1)\psi_m(\mathbf{r}) \\ &= \sum_{m=1}^{d}\sum_{p=1}^{d}\Gamma(T_2)_{mn}\Gamma(T_1)_{pm}\psi_p(\mathbf{r}) \\ &= \sum_{p=1}^{d}\Gamma(T_1T_2)_{pn}\psi_p(\mathbf{r}). \end{aligned}$$

Example II *Some basis functions of the crystallographic point group* D_4
The functions $\psi_1(\mathbf{r}) = x, \psi_2(\mathbf{r}) = z$ provide a basis for the representation $\mathbf{\Gamma}$ of D_4 that has been constructed in Example I above, as can be verified by inspection. (This set has been deduced by a method that will be described in detail in Chapter 5, Section 1.)

Theorem I The eigenfunctions of a d-fold degenerate eigenvalue ϵ of the time-independent Schrödinger equation

$$H(\mathbf{r})\psi(\mathbf{r}) = \epsilon\psi(\mathbf{r})$$

form a basis for a d-dimensional representation of the group of the Schrödinger equation $\mathcal{G}$.

Proof Let $\psi_1(\mathbf{r}), \psi_2(\mathbf{r}), \ldots, \psi_d(\mathbf{r})$ be a set of linearly independent eigenfunctions of $H(\mathbf{r})$ with eigenvalue ϵ, so that

$$H(\mathbf{r})\psi_n(\mathbf{r}) = \epsilon\psi_n(\mathbf{r}), \quad n = 1, 2, \ldots, d,$$

and any other eigenfunction of $H(\mathbf{r})$ with eigenvalue ϵ is a linear combination of $\psi_1(\mathbf{r}), \psi_2(\mathbf{r}), \ldots, \psi_d(\mathbf{r})$. For any transformation T of the group of the Schrödinger equation, Equation (1.23) implies that

$$H(\mathbf{r})\{P(T)\psi_n(\mathbf{r})\} = P(T)\{H(\mathbf{r})\psi_n(\mathbf{r})\} = \epsilon\{P(T)\psi_n(\mathbf{r})\},$$

demonstrating that $P(T)\psi_n(\mathbf{r})$ is also an eigenfunction of $H(\mathbf{r})$ with eigenvalue ϵ, so that $P(T)\psi_n(\mathbf{r})$ may be written in the form

$$P(T)\psi_n(\mathbf{r}) = \sum_{m=1}^{d}\Gamma(T)_{mn}\psi_m(\mathbf{r}), \quad n = 1, 2, \ldots, d. \tag{1.27}$$

At this stage the $\Gamma(T)_{mn}$ are merely a set of coefficients with the m, n and T dependence explicitly displayed. For each T the set $\Gamma(T)_{mn}$ can be arranged to form a $d \times d$ matrix $\mathbf{\Gamma}(T)$. It will now be shown that

$$\Gamma(T_1T_2)_{mn} = \sum_{p=1}^{d} \Gamma(T_1)_{mp}\Gamma(T_2)_{pn} \tag{1.28}$$

for any two transformations T_1 and T_2 of $\mathcal{G}$, thereby demonstrating that the matrices $\mathbf{\Gamma}(T)$ do actually form a representation of $\mathcal{G}$. Equation (1.27) then implies that the eigenfunctions $\psi_1(\mathbf{r}), \psi_2(\mathbf{r}), \ldots, \psi_d(\mathbf{r})$ form a basis for this representation.

From Equation (1.27), with T replaced by T_1, T_2 and T_1T_2 in turn,

$$P(T_1)\psi_p(\mathbf{r}) = \sum_{m=1}^{d} \Gamma(T_1)_{mp}\psi_m(\mathbf{r}), \tag{1.29}$$

$$P(T_2)\psi_n(\mathbf{r}) = \sum_{p=1}^{d} \Gamma(T_2)_{pn}\psi_p(\mathbf{r}), \tag{1.30}$$

$$P(T_1T_2)\psi_n(\mathbf{r}) = \sum_{m=1}^{d} \Gamma(T_1T_2)_{mn}\psi_m(\mathbf{r}). \tag{1.31}$$

From Equations (1.29) and (1.30)

$$P(T_1)P(T_2)\psi_n(\mathbf{r}) = \sum_{m=1}^{d}\sum_{p=1}^{d} \Gamma(T_1)_{mp}\Gamma(T_2)_{pn}\psi_m(\mathbf{r}), \tag{1.32}$$

and, as $P(T_1)P(T_2)\psi_n(\mathbf{r}) = P(T_1T_2)\psi_n(\mathbf{r})$ by Equation (1.22), the right hand sides of Equations (1.31) and (1.32) must be equal. As the functions $\psi_1(\mathbf{r})$, $\psi_2(\mathbf{r})$, ..., $\psi_d(\mathbf{r})$ have been assumed to be linearly independent, Equation (1.28) follows on equating coefficients of each $\psi_m(\mathbf{r})$.

This theorem implies that each energy eigenvalue can be labelled by a representation of the group of the Schrödinger equation. In Chapter 10 it will be shown that the familiar categorization of electronic states of an atom into "s-states", "p-states", "d-states" etc. is actually just a special case of this type of description. More precisely, every s-state eigenfunction is a basis function of particular representation of the group of rotations in three dimensions, the p-state eigenfunctions are basis functions of another representation of that group, and so on.

Having established a prima facie case that groups and their representations play a significant role in the quantum mechanical study of physical systems, the next chapters will be devoted to a detailed examination of the structure of groups and the theory of their representations. So far only a brief indication has been given of what can be achieved, but the ensuing chapters will show that the group theoretical approach is capable of dealing with a very wide range of profound and detailed questions.

Chapter 2

The Structure of Groups

1 Some elementary considerations

This section will be devoted to some immediate consequences of the definition of a group that was given in Chapter 1, Section 1. As many statements will be made about the contents of various sets, it is convenient to introduce an abbreviated notation in which "$T \in \mathcal{S}$" means "the element T is a member of the set $\mathcal{S}$" and "$T \notin \mathcal{S}$" means "the element T is not a member of the set $\mathcal{S}$".

The associative law of Equation (1.1) implies that in any product of three or more elements no ambiguity arises if the brackets are removed completely. Moreover, they can be inserted freely around any chosen subset or subsets of elements in the product, provided of course that the order of elements is unchanged. The proof that

$$(T_1T_2)^{-1} = T_2^{-1}T_1^{-1} \tag{2.1}$$

for any $T_1, T_2 \in \mathcal{G}$ provides some examples of this, for

$$\begin{aligned}(T_2^{-1}T_1^{-1})(T_1T_2) &= T_2^{-1}(T_1^{-1}T_1)T_2 = T_2^{-1}ET_2 \\ &= T_2^{-1}(ET_2) = T_2^{-1}T_2 = E,\end{aligned}$$

there being a similar argument for $(T_1T_2)(T_2^{-1}T_1^{-1})$.

Definition *Subgroup*
A subset $\mathcal{S}$ of a group $\mathcal{G}$ that is itself a group with the same multiplication operation as $\mathcal{G}$ is called a "subgroup" of $\mathcal{G}$.

By convention, a set may be considered to be a subset of itself, so $\mathcal{G}$ can be regarded as being a subgroup of itself. All other subgroups of $\mathcal{G}$ are called *proper subgroups*. Obviously the identity E must be a member of every subgroup of $\mathcal{G}$. Indeed one subgroup of $\mathcal{G}$ is the set $\{E\}$ consisting only of E. It will be shown in Section 4 that if g and s are the orders of $\mathcal{G}$ and $\mathcal{S}$ respectively, then g/s must be an integer.

A concise criterion for a subset of a group to be a subgroup is provided by the following theorem.

Theorem I If $\mathcal{S}$ is a subset of a group $\mathcal{G}$ such that $S'S^{-1} \in \mathcal{S}$ for any two elements S and S' of $\mathcal{S}$, then $\mathcal{S}$ is a subgroup of $\mathcal{G}$.

Proof It has only to be verified that the group axioms (a), (c) and (d) are satisfied by $\mathcal{S}$, axiom (b) being automatically obeyed for any subset of $\mathcal{G}$. Putting $S' = S$ gives $S'S^{-1} = E$, so $E \in \mathcal{S}$ and hence axiom (c) is satisfied. Putting $S' = E$ gives $S'S^{-1} = S^{-1}$, so $S^{-1} \in \mathcal{S}$, thereby fulfilling axiom (d). Finally, as $S^{-1} \in \mathcal{S}$, $S'(S^{-1})^{-1} = S'S \in \mathcal{S}$, so (a) is also true.

Example I *Subgroups of the crystallographic point group* D_4
The group D_4 defined in Chapter 1, Section 2 has the following subgroups:

(a) $s = 1$ (i.e. $g/s = 8$): $\{E\}$;

(b) $s = 2$ (i.e. $g/s = 4$): $\{E, C_{2x}\}$, $\{E, C_{2y}\}$, $\{E, C_{2z}\}$, $\{E, C_{2c}\}$, $\{E, C_{2d}\}$;

(c) $s = 4$ (i.e. $g/s = 2$): $\{E, C_{2x}, C_{2y}, C_{2z}\}$, $\{E, C_{2y}, C_{4y}, C_{4y}^{-1}\}$, $\{E, C_{2y}, C_{2c}, C_{2d}\}$;

(d) $s = 8$ (i.e. $g/s = 1$): $\{E, C_{2x}, C_{2y}, C_{2z}, C_{4y}, C_{4y}^{-1}, C_{2c}, C_{2d}\}$.

The following theorem displays an interesting property of multiplication in a group.

Theorem II For any fixed element T' of a group $\mathcal{G}$, the sets $\{T'T; T \in \mathcal{G}\}$ and $\{TT'; T \in \mathcal{G}\}$ both contain every element of $\mathcal{G}$ once and only once. (Here $\{T'T; T \in \mathcal{G}\}$ denotes the set of elements $T'T$ where T varies over the whole of $\mathcal{G}$. For example, in the special case in which $\mathcal{G}$ is a finite group of order g with elements $T_1, T_2, \ldots, T_g$ and $T' = T_n$, this set consists of $T_nT_1, T_nT_2, \ldots, T_nT_g$. The interpretation of $\{TT'; T \in \mathcal{G}\}$ is similar. The theorem is often called the "Rearrangement Theorem", as it asserts that each of the two sets $\{T'T; T \in \mathcal{G}\}$ and $\{TT'; T \in \mathcal{G}\}$ merely consists of the elements of $\mathcal{G}$ rearranged in order.)

Proof An explicit proof will be given for the set $\{T'T; T \in \mathcal{G}\}$, the proof for the other set being similar.

If T'' is any element of $\mathcal{G}$, then with T defined by $T = (T')^{-1}T''$ it follows that $T'T = T''$. Thus $\{T'T; T \in \mathcal{G}\}$ certainly contains every element of $\mathcal{G}$ at least once. Now suppose that $\{T'T; T \in \mathcal{G}\}$ contains some element of $\mathcal{G}$ twice (or more), i.e. for some $T_1, T_2 \in \mathcal{G}$, $T'T_1 = T'T_2$, but $T_1 \neq T_2$. However, these statements are inconsistent, for premultiplying the first by $(T')^{-1}$ gives $T_1 = T_2$, so no element of $\mathcal{G}$ appears more than once in $\{T'T; T \in \mathcal{G}\}$.

The Rearrangement Theorem implies that in the multiplication table of a finite group every element of the group appears *once and only once* in every

row, and *once and only once* in every *column*. This provides a useful check on the computation of the multiplication table. Tables 1.1 and 1.2 exemplify these properties.

2 Classes

Whereas in ordinary everyday language the word "class" is often synonymous with the word "set", in the context of group theory a class is defined to be a special type of set. In fact it is a subset of a group having a certain property which causes it to play an important role in representation theory, as will be shown in Chapter 4.

As a preliminary it is necessary to introduce the idea of "conjugate elements" of a group.

Definition *Conjugate elements*
An element T' of a group $\mathcal{G}$ is said to be "conjugate" to another element T of $\mathcal{G}$ if there exists an element X of $\mathcal{G}$ such that

$$T' = XTX^{-1}. \tag{2.2}$$

If T' is conjugate to T, then T is conjugate to T', as Equation (2.2) can be rewritten as $T = X^{-1}T'(X^{-1})^{-1}$. Moreover, if T, T' and T'' are three elements of $\mathcal{G}$ such that T' and T'' are both conjugate to T, then T' is conjugate to T''. This follows because there exist elements X and Y of $\mathcal{G}$ such that $T' = XTX^{-1}$ and $T'' = YTY^{-1}$, so that $T' = X(Y^{-1}T''Y)X^{-1} = (XY^{-1})T''(XY^{-1})^{-1}$ (by Equation (2.1)), which has the form of Equation (2.2) as $XY^{-1} \in \mathcal{G}$. It is therefore permissible to talk of a set of *mutually* conjugate elements.

Definition *Class*
A class of a group $\mathcal{G}$ is a set of mutually conjugate elements of $\mathcal{G}$. (For extra precision this is sometimes called a "conjugacy class".)

A class can be constructed from any $T \in \mathcal{G}$ by forming the set of products XTX^{-1} for every $X \in \mathcal{G}$, retaining only the distinct elements. This class contains T itself as $T = ETE^{-1}$.

Example I *Classes of the crystallographic point group D_4*
For the group D_4 this procedure when applied to C_{2x} gives (on using Table 1.2):

$$\begin{aligned} XC_{2x}X^{-1} &= C_{2x} \text{ for } X = E, C_{2x}, C_{2y}, C_{2z}, \\ XC_{2x}X^{-1} &= C_{2z} \text{ for } X = C_{4y}^{-1}, C_{4y}, C_{2c}, C_{2d}. \end{aligned}$$

Thus $\{C_{2x}, C_{2z}\}$ is one of the classes of D_4. The same class would have been found if the procedure had been applied to C_{2z}. D_4 has four other classes,

namely $\{E\}$, $\{C_{2y}\}$, $\{C_{4y}, C_{4y}^{-1}\}$ and $\{C_{2c}, C_{2d}\}$, which may be deduced in a similar way.

The properties of classes are conveniently summarized in the following three theorems.

Theorem I

(a) Every element of a group $\mathcal{G}$ is a member of some class of $\mathcal{G}$.

(b) No element of $\mathcal{G}$ can be a member of two different classes of $\mathcal{G}$.

(c) The identity E of $\mathcal{G}$ always forms a class on its own.

Proof

(a) As noted above, for any $T \in \mathcal{G}$, $ETE^{-1} = T$, so that T is in the class constructed from itself.

(b) Suppose that $T \in \mathcal{G}$ is a member of a class containing T' and is also a member of a class containing T''. Then T is conjugate to T' and T'', so T' and T'' must be conjugate and must therefore be in the same class.

(c) For any $X \in \mathcal{G}$, $XEX^{-1} = XX^{-1} = E$, so E forms a class on its own.

Theorem II If $\mathcal{G}$ is an *Abelian* group, *every* element of $\mathcal{G}$ forms a class on its own.

Proof For any T and X of an Abelian group $\mathcal{G}$

$$XTX^{-1} = XX^{-1}T = ET = T,$$

so T forms a class on its own.

Theorem III If $\mathcal{G}$ is a group consisting entirely of pure rotations, no class of $\mathcal{G}$ contains both proper and improper rotations. Moreover, in each class of proper rotations all the rotations are through the same angle. Similarly, in each class of improper rotations the proper parts are all through the same angle.

Proof If T and T' are two pure rotations in the same class, Equations (1.4) and (2.2) imply that $\mathbf{R}(T') = \mathbf{R}(X)\mathbf{R}(T)\mathbf{R}(X)^{-1}$, so that

$$\det \mathbf{R}(T') = \det \mathbf{R}(T) \tag{2.3}$$

and

$$\operatorname{tr} \mathbf{R}(T') = \operatorname{tr} \mathbf{R}(T) \tag{2.4}$$

(see Appendix A). Equation (2.3) shows that T and T' are either both proper or are both improper. Moreover, for any proper rotation T through an angle θ (in the right- or left-hand screw sense) $\mathrm{tr}\,\mathbf{R}(T) = 1 + 2\cos\theta$ (cf. Equation (10.4)). Equation (2.4) then implies that all proper rotations in a class are through the same angle θ. Finally, by expressing any improper rotation T as the product of the spatial inversion operator I with a proper rotation through an angle θ, it follows that $\mathrm{tr}\mathbf{R}(T) = -\{1+2\cos\theta\}$, so all proper parts involved in a class are through the same angle θ.

It should be noted that the converse of the last theorem is not necessarily true, in that there is no requirement for all rotations of the same type to be in the same class. Indeed, in the above example of the point group D_4, the proper rotations C_{2x} and C_{2y} are in different classes, even though they are rotations through the same angle π.

3 Invariant subgroups

The main object of this and the following section is to introduce two concepts that are involved in the construction of factor groups.

Definition *Invariant subgroup*
A subgroup $\mathcal{S}$ of a group $\mathcal{G}$ is said to be an "invariant" subgroup if

$$XSX^{-1} \in \mathcal{S} \tag{2.5}$$

for every $S \in \mathcal{S}$ and every $X \in \mathcal{G}$.

Invariant subgroups are sometimes called "normal subgroups" or "normal divisors". Because of the occurrence of the same forms in Equation (2.2) and Condition (2.5), there is a close connection between invariant subgroups and classes.

Theorem I A subgroup $\mathcal{S}$ of a group $\mathcal{G}$ is an *invariant* subgroup if and only if $\mathcal{S}$ consists entirely of *complete* classes of $\mathcal{G}$.

Proof Suppose first that $\mathcal{S}$ is an invariant subgroup of $\mathcal{G}$. Then if S is any member of $\mathcal{S}$ and T is any member of the same class of $\mathcal{G}$ as S, by Equation (2.2) there exists an element X of $\mathcal{G}$ such that $T = XSX^{-1}$. Condition (2.5) then implies that $T \in \mathcal{S}$, so the whole class of $\mathcal{G}$ containing S is contained in $\mathcal{S}$.

Now suppose that $\mathcal{S}$ consists entirely of complete classes of $\mathcal{G}$, and let S be any member of $\mathcal{S}$. Then the set of products XSX^{-1} for all $X \in \mathcal{G}$ forms the class containing S, which by assumption is contained in $\mathcal{S}$. Thus $XSX^{-1} \in \mathcal{S}$ for all $S \in \mathcal{S}$ and $X \in \mathcal{G}$, so $\mathcal{S}$ is an invariant subgroup of $\mathcal{G}$.

This theorem provides a very easy method of determining which of the

subgroups of a group are invariant when the classes have been previously calculated.

Example I *Invariant subgroups of the crystallographic point group D_4*
For the crystallographic point group D_4 it follows immediately from the lists of subgroups and classes given in Sections 1 and 2 that the invariant subgroups are $\{E\}$, $\{E, C_{2y}\}$, $\{E, C_{2x}, C_{2y}, C_{2z}\}$, $\{E, C_{2y}, C_{4y}, C_{4y}^{-1}\}$, $\{E, C_{2y}, C_{2c}, C_{2d}\}$, and D_4 itself. (The subgroup $\{E, C_{2x}\}$ is not an invariant subgroup as C_{2x} is part of a class $\{C_{2x}, C_{2z}\}$ that is not wholly contained in the subgroup. The same is true of $\{E, C_{2c}\}$ and $\{E, C_{2d}\}$.)

For every $\mathcal{G}$ the trivial subgroups $\{E\}$ and $\mathcal{G}$ are both invariant subgroups.

4 Cosets

Definition *Coset*
Let $\mathcal{S}$ be a subgroup of a group $\mathcal{G}$. Then, for any fixed $T \in \mathcal{G}$ (which may or may not be a member of $\mathcal{S}$), the set of elements ST, where S varies over the whole of $\mathcal{S}$, is called the "right coset" of $\mathcal{S}$ with respect to T, and is denoted by $\mathcal{S}T$. Similarly, the set of elements TS is called the "left coset" of $\mathcal{S}$ with respect to T and is denoted by $T\mathcal{S}$.

In particular, if $\mathcal{S}$ is a finite subgroup of order s with elements S_1, S_2, ..., S_s, then $\mathcal{S}T$ is the set of s elements $S_1T, S_2T, \ldots, S_sT$, and $T\mathcal{S}$ is the set of s elements $TS_1, TS_2, \ldots, TS_s$. In the following discussions two sets will be said to be identical if they merely contain the same elements, the ordering of the elements within the sets being immaterial.

Example I *Some cosets of the crystallographic point group D_4*
Let $\mathcal{G}$ be D_4 and let $\mathcal{S} = \{E, C_{2x}\}$. Then from Table 1.2 the right cosets are

$$\begin{aligned} \mathcal{S}E = \mathcal{S}C_{2x} &= \{E, C_{2x}\}, \\ \mathcal{S}C_{2y} = \mathcal{S}C_{2z} &= \{C_{2y}, C_{2z}\}, \\ \mathcal{S}C_{4y} = \mathcal{S}C_{2d} &= \{C_{4y}, C_{2d}\}, \\ \mathcal{S}C_{4y}^{-1} = \mathcal{S}C_{2c} &= \{C_{4y}^{-1}, C_{2e}\}, \end{aligned}$$

and the left cosets are

$$\begin{aligned} E\mathcal{S} = C_{2x}\mathcal{S} &= \{E, C_{2x}\}, \\ C_{2y}\mathcal{S} = C_{2z}\mathcal{S} &= \{C_{2y}, C_{2z}\}, \\ C_{4y}\mathcal{S} = C_{2c}\mathcal{S} &= \{C_{4y}, C_{2c}\}, \\ C_{4y}^{-1}\mathcal{S} = C_{2d}\mathcal{S} &= \{C_{4y}^{-1}, C_{2d}\}. \end{aligned}$$

It should be noted that $C_{4y}\mathcal{S} \neq \mathcal{S}C_{4y}$ and $C_{4y}^{-1}\mathcal{S} \neq \mathcal{S}C_{4y}^{-1}$.

This example shows that the right and left cosets $\mathcal{S}T$ and $T\mathcal{S}$ formed from the same element $T \in \mathcal{G}$ are not necessarily identical. The properties of cosets are summarized in the following two theorems. The first theorem is stated for right cosets, but every statement applies equally to left cosets. It is worth while checking that the above example of the point group D_4 does satisfy all the assertions of this theorem.

Theorem I

(a) If $T \in \mathcal{S}$, then $\mathcal{S}T = \mathcal{S}$.

(b) If $T \notin \mathcal{S}$, then $\mathcal{S}T$ is not a subgroup of $\mathcal{G}$.

(c) Every element of $\mathcal{G}$ is a member of some right coset.

(d) Any two elements ST and $S'T$ of $\mathcal{S}T$ are different, provided that $S \neq S'$. In particular, if $\mathcal{S}$ is a finite subgroup of order s, $\mathcal{S}T$ contains s different elements.

(e) Two right cosets of $\mathcal{S}$ are either identical or have no elements in common.

(f) If $T' \in \mathcal{S}T$, then $\mathcal{S}T' = \mathcal{S}T$.

(g) If $\mathcal{G}$ is a finite group of order g and $\mathcal{S}$ has order s, then the number of distinct right cosets is g/s.

Proof

(a) If $T \in \mathcal{S}$, the Rearrangement Theorem of Section 1 applied to $\mathcal{S}$ considered as a group shows that $\mathcal{S}T$ is merely a rearrangement of $\mathcal{S}$.

(b) If $\mathcal{S}T$ is a subgroup of $\mathcal{G}$, it must contain the identity E, so there must exist an element $S \in \mathcal{S}$ such that $ST = E$. This implies $T = S^{-1}$, so $T \in \mathcal{S}$. Thus if $T \notin \mathcal{S}$, $\mathcal{S}T$ cannot be a subgroup of $\mathcal{G}$.

(c) For any $T \in \mathcal{S}$, as $T = ET$ and $E \in \mathcal{S}$, it follows that $T \in \mathcal{S}T$.

(d) Suppose that $ST = S'T$ and $S \neq S'$. Post-multiplying by T^{-1} gives $S = S'$, a contradiction.

(e) Suppose that $\mathcal{S}T$ and $\mathcal{S}T'$ are two right cosets with a common element. It will be shown that $\mathcal{S}T = \mathcal{S}T'$. Let $ST = S'T'$ be the common element of $\mathcal{S}T$ and $\mathcal{S}T'$. Here $S, S' \in \mathcal{S}$. Then $T'T^{-1} = (S')^{-1}S$, so $T'T^{-1} \in \mathcal{S}$, and hence by (a) $\mathcal{S}(T'T^{-1}) = \mathcal{S}$. As $\mathcal{S}(T'T^{-1})$ is the set of elements of the form $ST'T^{-1}$, the set obtained from this by post-multiplying each member by T consists of the elements ST', that is, it is the coset $\mathcal{S}T'$. Thus $\mathcal{S}T = \mathcal{S}T'$.

(f) As in (c), $T' \in \mathcal{S}T'$. If $T \in \mathcal{S}T'$ then $\mathcal{S}T'$ and $\mathcal{S}T$ have a common element and must therefore be identical by (e).

(g) Suppose that there are M distinct right cosets of $\mathcal{S}$. By (d) each contains s different elements, so the collection of distinct cosets contains Ms different elements of $\mathcal{G}$. But by (c) every element of $\mathcal{G}$ is in this collection of distinct cosets, so $Ms = g$.

The property (f) is particularly important. It shows that the same coset is formed starting from *any* member of the coset. All members of a coset therefore appear on an equal footing, so that *any* member of the coset can be taken as the "coset representative" that labels the coset and from which the coset can be constructed. For example, for the right coset $\{C_{4y}, C_{2d}\}$ of the point group D_4, the coset representatives could equally well be chosen to be C_{4y} or C_{2d}. As the number of distinct right cosets is necessarily a positive integer, property (g) demonstrates that s must divide g, as was mentioned in Section 1.

Theorem II The right and left cosets of a subgroup $\mathcal{S}$ of a group $\mathcal{G}$ are *identical* (i.e. $\mathcal{S}T = T\mathcal{S}$ for all $T \in \mathcal{G}$) if and only if $\mathcal{S}$ is an *invariant* subgroup of $\mathcal{G}$.

Proof Suppose that $\mathcal{S}$ is an invariant subgroup. It will be shown that if $T' \in \mathcal{S}T$ then $T' \in T\mathcal{S}$. (A similar argument proves that if $T' \in T\mathcal{S}$ then $T' \in \mathcal{S}T$, so, on combining the two, it follows that $\mathcal{S}T = T\mathcal{S}$.) If $T' \in \mathcal{S}T$ there exists an element S of $\mathcal{S}$ such that $T' = ST$. Then $T^{-1}T' = T^{-1}ST$, which is a member of $\mathcal{S}$ as $\mathcal{S}$ is an invariant subgroup. Thus $T^{-1}T' \in \mathcal{S}$, so $T' = T(T^{-1}T')$ must be a member of $T\mathcal{S}$.

Now suppose that $\mathcal{S}T = T\mathcal{S}$ for every $T \in \mathcal{G}$. This implies that for any $S \in \mathcal{S}$ and any $T \in \mathcal{G}$ there exists an $S' \in \mathcal{S}$ such that $TS = S'T$, so $TST^{-1} = S'$ and hence $TST^{-1} \in \mathcal{S}$. Thus $\mathcal{S}$ is an invariant subgroup of $\mathcal{G}$.

Of course, in the above example concerning the point group D_4, the subgroup $\mathcal{S} = \{E, C_{2x}\}$ was carefully chosen so as *not* to be an invariant subgroup, in order to demonstrate that right and left cosets are not always identical.

5 Factor groups

Let $\mathcal{S}$ be an *invariant* subgroup of a group $\mathcal{G}$. Each right coset of $\mathcal{S}$ can be considered to be an "element" of the set of distinct right cosets of $\mathcal{S}$, the internal structure of each coset now being disregarded. With the following definition of the product of two right cosets, the set of cosets then forms a group called a "factor group".

Definition *Product of right cosets*
The product of two right cosets $\mathcal{S}T_1$ and $\mathcal{S}T_2$ of an *invariant* subgroup $\mathcal{S}$ is defined by

$$\mathcal{S}T_1.\mathcal{S}T_2 = \mathcal{S}(T_1T_2). \tag{2.6}$$

Proof of consistency It will be shown that Equation (2.6) provides a meaningful definition, in that, if alternative coset representatives are chosen for the cosets on the left-hand side of the equation, then the coset on the right-hand side remains unchanged. Suppose that T_1' and T_2' are alternative coset representatives for $\mathcal{S}T_1$ and $\mathcal{S}T_2$ respectively, so that $T_1' \in \mathcal{S}T_1$ and $T_2' \in \mathcal{S}T_2$. It has to be proved that $\mathcal{S}(T_1'T_2') = \mathcal{S}(T_1T_2)$. As $T_1' \in \mathcal{S}T_1$ and $T_2' \in \mathcal{S}T_2$, there exist $S, S' \in \mathcal{S}$ such that $T_1' = ST_1$ and $T_2' = S'T_2'$. Then $T_1'T_2' = ST_1S'T_2$. But $T_1S' \in T_1\mathcal{S}$, so, as $\mathcal{S}$ is an invariant subgroup, $T_1S' \in \mathcal{S}T_1$. Consequently there exists an $S'' \in \mathcal{S}$ such that $T_1S' = S''T_1$. Then $T_1'T_2' = (SS'')(T_1T_2)$, so that $T_1'T_2' \in \mathcal{S}(T_1T_2)$ and hence, by property (f) of the first theorem of Section 4, $\mathcal{S}(T_1'T_2') = \mathcal{S}(T_1T_2)$.

Theorem I The set of right cosets of an *invariant* subgroup $\mathcal{S}$ of a group $\mathcal{G}$ forms a group, with Equation (2.6) defining the group multiplication operation. This group is called a "factor group" and is denoted by $\mathcal{G}/\mathcal{S}$.

Proof It has only to be verified that the four group axioms are satisfied.

(a) By Equation (2.6), the product of any two right cosets of $\mathcal{S}$ is itself a right coset of $\mathcal{S}$ and is therefore a member of $\mathcal{G}/\mathcal{S}$.

(b) The associative law is valid for coset multiplication because, if $\mathcal{S}T$, $\mathcal{S}T'$ and $\mathcal{S}T''$ are any three right cosets,

$$(\mathcal{S}T.\mathcal{S}T').\mathcal{S}T'' = \mathcal{S}(TT').\mathcal{S}T'' = \mathcal{S}((TT')T'')$$

and

$$\mathcal{S}T.(\mathcal{S}T'.\mathcal{S}T'') = \mathcal{S}T.\mathcal{S}(T'T'') = \mathcal{S}(T(T'T'')),$$

where the two cosets on the right-hand sides are equal by virtue of the associative law $(TT')T'' = T(T'T'')$ for $\mathcal{G}$.

(c) The identity element of $\mathcal{G}/\mathcal{S}$ is $\mathcal{S}E(=\mathcal{S})$, as for any right coset

$$\mathcal{S}E.\mathcal{S}T = \mathcal{S}(ET) = \mathcal{S}T = \mathcal{S}(TE) = \mathcal{S}T.\mathcal{S}E.$$

(d) The inverse of $\mathcal{S}T$ is $\mathcal{S}(T^{-1})$, as

$$\mathcal{S}T.\mathcal{S}(T^{-1}) = \mathcal{S}(TT^{-1}) = \mathcal{S}E = \mathcal{S}(T^{-1}T) = \mathcal{S}(T^{-1}).\mathcal{S}T.$$

The coset $\mathcal{S}(T^{-1})$ is a member of $\mathcal{G}/\mathcal{S}$ as $T^{-1} \in \mathcal{G}$.

If $\mathcal{G}$ is a finite group of order g and $\mathcal{S}$ has order s, part (g) of the first theorem of Section 4 shows that there are g/s distinct right cosets. Thus $\mathcal{G}/\mathcal{S}$ is a group of order g/s with elements $\mathcal{S}T_1, \mathcal{S}T_2, \ldots, \mathcal{S}T_s$, $(T_1, T_2, \ldots, T_s$ being a set of coset representatives). As $\mathcal{S}$ itself is one of the cosets, one can take $T_1 = E$.

	$\mathcal{S}E$	$\mathcal{S}C_{2x}$	$\mathcal{S}C_{4y}$	$\mathcal{S}C_{2c}$
$\mathcal{S}E$	$\mathcal{S}E$	$\mathcal{S}C_{2x}$	$\mathcal{S}C_{4y}$	$\mathcal{S}C_{2c}$
$\mathcal{S}C_{2x}$	$\mathcal{S}C_{2x}$	$\mathcal{S}E$	$\mathcal{S}C_{2c}$	$\mathcal{S}C_{4y}$
$\mathcal{S}C_{4y}$	$\mathcal{S}C_{4y}$	$\mathcal{S}C_{2c}$	$\mathcal{S}E$	$\mathcal{S}C_{2x}$
$\mathcal{S}C_{2c}$	$\mathcal{S}C_{2c}$	$\mathcal{S}C_{4y}$	$\mathcal{S}C_{2x}$	$\mathcal{S}E$

Table 2.1: Multiplication table for the factor group $\mathcal{G}/\mathcal{S}$, where $\mathcal{G}$ is the crystallographic point group D_4 and $\mathcal{S} = \{E, C_{2y}\}$.

Example I *A factor group formed from the crystallographic point group D_4*
Let $\mathcal{G}$ be D_4 and let $\mathcal{S} = \{E, C_{2y}\}$, which is an invariant subgroup of $\mathcal{G}$ (see Example I of Section 3). Then $\mathcal{G}/\mathcal{S}$ is a group of order 4 with elements

$$\begin{aligned} \mathcal{S}E &= \mathcal{S}C_{2y} &&= \{E, C_{2y}\}, \\ \mathcal{S}C_{2x} &= \mathcal{S}SC_{2z} &&= \{C_{2x}, C_{2z}\}, \\ \mathcal{S}C_{4y} &= \mathcal{S}C_{4y}^{-1} &&= \{C_{4y}, C_{4y}^{-1}\}, \\ \mathcal{S}C_{2c} &= \mathcal{S}C_{2d} &&= \{C_{2c}, C_{2d}\}, \end{aligned}$$

whose multiplication table is given in Table 2.1. (Here it should be noted for example that $C_{2x}C_{4y} = C_{2d}$, so $\mathcal{S}C_{2x}.\mathcal{S}C_{4y} = \mathcal{S}C_{2d} = \mathcal{S}C_{2c}$).

6 Homomorphic and isomorphic mappings

Let $\mathcal{G}$ and $\mathcal{G}'$ be two groups. A "mapping" ϕ of $\mathcal{G}$ onto $\mathcal{G}'$ is simply a rule by which each element T of $\mathcal{G}$ is assigned to some element $T' = \phi(T)$ of $\mathcal{G}'$, with every element of $\mathcal{G}'$ being the "image" of at least one element of $\mathcal{G}$. If ϕ is a *one-to-one* mapping, that is, if each element T' of $\mathcal{G}'$ is the image of *only one* element T of $\mathcal{G}$, then the inverse mapping ϕ^{-1} of $\mathcal{G}'$ onto $\mathcal{G}$ may be defined by $\phi^{-1}(T') = T$ if and only if $T' = \phi(T)$.

Definition *Homomorphic mapping of a group $\mathcal{G}$ onto a group $\mathcal{G}'$*
If ϕ is a mapping of a group $\mathcal{G}$ onto a group $\mathcal{G}'$ such that

$$\phi(T_1)\phi(T_2) = \phi(T_1T_2) \tag{2.7}$$

for all $T_1, T_2 \in \mathcal{G}$, then ϕ is said to be a "homomorphic" mapping.

On the right-hand side of Equation (2.7) the product of T_1 with T_2 is evaluated using the group multiplication operation for $\mathcal{G}$, whereas on the left-hand side the product of $\phi(T_1)$ with $\phi(T_2)$ is obtained from the group multiplication operation for $\mathcal{G}'$. Although these operations may be different, there is no need to introduce any special notations to distinguish between them, because the relevant operation can always be deduced from the context and there is really no possibility of confusion.

Example I *A homomorphic mapping of the point group D_4*
Let $\mathcal{G}$ be D_4 and let $\mathcal{G}'$ be the group of order 2 with elements $+1$ and -1,

with ordinary multiplication as the group multiplication operation. Then

$$\begin{aligned} \phi(E) = \phi(C_{2y}) = \phi(C_{2x}) = \phi(C_{2z}) &= +1, \\ \phi(C_{4y}) = \phi(C_{4y}^{-1}) = \phi(C_{2c}) = \phi(C_{2d}) &= -1, \end{aligned}$$

is a homomorphic mapping of $\mathcal{G}$ onto $\mathcal{G}'$, as may be confirmed by examination of Table 1.2. For example, $\phi(C_{2x})\phi(C_{2c}) = (+1)(-1) = -1$, while Table 1.2 gives $\phi(C_{2x}C_{2c}) = \phi(C_{4y}^{-1}) = -1$.

Clearly, if g and g' are the orders of $\mathcal{G}$ and $\mathcal{G}'$ respectively, then $g \geq g'$. Actually, the First Homomorphism Theorem, which will be proved shortly, implies that if g and g' are both finite, then g/g' must be an integer. One major example of a homomorphic mapping has already been encountered in the concept of a representation of a group. Indeed, the definition in Chapter 1, Section 4 can now be rephrased as follows:

Definition *Representation of a group $\mathcal{G}$*
If there exists a *homomorphic* mapping of a group $\mathcal{G}$ onto a group of non-singular $d \times d$ matrices $\mathbf{\Gamma}(T)$ with matrix multiplication as the group multiplication operation, then the group of matrices $\mathbf{\Gamma}(T)$ forms a d-dimensional representation $\mathbf{\Gamma}$ of $\mathcal{G}$.

There is no requirement in the definition of a homomorphic mapping that the mapping should be one-to-one. However, as such mappings are particularly important, they are given a special name:

Definition *Isomorphic mapping of a group $\mathcal{G}$ onto a group $\mathcal{G}'$*
If ϕ is a *one-to-one* mapping of a group $\mathcal{G}$ onto a group $\mathcal{G}'$ of the same order such that

$$\phi(T_1)\phi(T_2) = \phi(T_1T_2)$$

$T_1, T_2 \in \mathcal{G}$, then ϕ is said to be an "isomorphic" mapping.

In the case of representations, if the homomorphic mapping is actually isomorphic, then the representation is said to be "faithful".

Clearly, if ϕ is an isomorphic mapping of $\mathcal{G}$ onto $\mathcal{G}'$, then the inverse mapping ϕ^{-1} is an isomorphic mapping of $\mathcal{G}'$ onto $\mathcal{G}$. (There is no analogous result for general homomorphic mappings, as ϕ^{-1} is only well defined when ϕ is a one-to-one mapping.)

Although two isomorphic groups may differ in the nature of their elements, they have the same structure of subgroups, cosets, classes, and so on. Most important of all, isomorphic groups necessarily have identical representations.

The following theorem clarifies various aspects of homomorphic mappings. As it is the first of a series of such theorems, it is often called the "First Homomorphism Theorem", but the others in the series will not be needed in this book.

Definition *Kernel $\mathcal{K}$ of a homomorphic mapping*
Let ϕ be a homomorphic mapping of a group $\mathcal{G}$ onto a group $\mathcal{G}'$. Then the set of elements $T \in \mathcal{G}$ such that $\phi(T) = E'$, the identity of $\mathcal{G}'$, is said to form the "kernel" $\mathcal{K}$ of the mapping.

Theorem I Let ϕ be a homomorphic mapping of $\mathcal{G}$ onto $\mathcal{G}'$, and let $\mathcal{K}$ be the kernel of this mapping. Then

(a) $\mathcal{K}$ is an invariant subgroup of $\mathcal{G}$;

(b) every element of the right coset $\mathcal{K}T$ maps onto the *same* element $\phi(T)$ of $\mathcal{G}'$, and the mapping θ thereby defined by

$$\theta(\mathcal{K}T) = \phi(T) \tag{2.8}$$

is a one-to-one mapping of the factor group $\mathcal{G}/\mathcal{K}$ onto $\mathcal{G}'$; and

(c) θ is an *isomorphic* mapping of $\mathcal{G}/\mathcal{K}$ onto $\mathcal{G}'$.

Proof See, for example, Chapter 2, Section 6, of Cornwell (1984).

One consequence of the theorem is that every element of $\mathcal{G}'$ is the image of the *same* number of elements of $\mathcal{G}$. This has the further implication that the mapping is an isomorphism if and only if $\mathcal{K}$ consists only of the identity E of $\mathcal{G}$.

In the special case in which $\mathcal{G}'$ is identical to $\mathcal{G}$ (so that ϕ is a mapping of $\mathcal{G}$ onto itself), an isomorphic mapping is known as an "automorphism". For each $X \in \mathcal{G}$ the mapping ϕ_X of $\mathcal{G}$ onto itself defined by

$$\phi_X(T) = XTX^{-1}$$

is an automorphism, as it is certainly one-to-one and

$$\phi_X(T_1)\phi_X(T_2) = (XT_1X^{-1})(XT_2X^{-1}) = X(T_1T_2)X^{-1} = \phi_X(T_1T_2)$$

for all $T_1, T_2 \in \mathcal{G}$. Such a mapping is called an "inner automorphism", and any automorphism that is not of this form is known as an "outer automorphism".

The whole theory of spin for electrons and other elementary particles in non-relativistic quantum mechanics is based on the following theorem.

Theorem II There exists a two-to-one homomorphic mapping of the group SU(2) onto the group SO(3). If $\mathbf{u} \in \mathrm{SU}(2)$ maps onto $\mathbf{R}(\mathbf{u}) \in \mathrm{SO}(3)$, then $\mathbf{R}(\mathbf{u}) = \mathbf{R}(-\mathbf{u})$, and the mapping may be chosen so that

$$R(\mathbf{u})_{jk} = \frac{1}{2}\mathrm{tr}\,\{\boldsymbol{\sigma}_j \mathbf{u} \boldsymbol{\sigma}_k \mathbf{u}^{-1}\} \tag{2.9}$$

for $j, k = 1, 2, 3$, where

$$\boldsymbol{\sigma}_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \boldsymbol{\sigma}_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \boldsymbol{\sigma}_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{2.10}$$

are the Pauli spin matrices. The kernel K of the mapping consists only of $\mathbf{1}_2$ and $-\mathbf{1}_2$.

Proof See, for example, Chapter 3, Section 5, of Cornwell (1984).

7 Direct products and semi-direct products of groups

Although the abstract construction of direct product groups appears at first sight rather artificial, a number of examples of groups having this structure occur naturally in physical problems.

Let $\mathcal{G}_1$ and $\mathcal{G}_2$ be any two groups, and suppose that E_1 and E_2 are the identities of $\mathcal{G}_1$ and $\mathcal{G}_2$ respectively. Consider the set of pairs (T_1, T_2), where $T_1 \in \mathcal{G}_1$ and $T_2 \in \mathcal{G}_2$, and define the product of two such pairs (T_1, T_2) and (T_1', T_2') by

$$(T_1, T_2)(T_1', T_2') = (T_1 T_1', T_2 T_2') \tag{2.11}$$

for all $T_1, T_1' \in \mathcal{G}_1$ and $T_2, T_2' \in \mathcal{G}_2$.

Theorem I The set of pairs (T_1, T_2) (for $T_1 \in \mathcal{G}_1$, $T_2 \in \mathcal{G}_2$) forms a group with Equation (2.11) as the group multiplication operation. This group is denoted by $\mathcal{G}_1 \otimes \mathcal{G}_2$, and is called the "direct product of $\mathcal{G}_1$ with $\mathcal{G}_2$".

Proof All that has to be verified is that the four group axioms of Chapter 1, Section 1, are satisfied. By Equation (2.11), the product of any two pairs of $\mathcal{G}_1 \otimes \mathcal{G}_2$ also a member of $\mathcal{G}_1 \otimes \mathcal{G}_2$, so axiom (a) is fulfilled. Axiom (b) is observed, as

$$\{(T_1, T_2)(T_1', T_2')\}(T_1'', T_2'') = ((T_1 T_1')T_1'', (T_2 T_2')T_2'')$$

and

$$(T_1, T_2)\{(T_1', T_2')(T_1'', T_2'')\} = ((T_1(T_1' T_1'')), (T_2(T_2' T_2''))),$$

the pairs on the right-hand sides being equal because the associative law applies to $\mathcal{G}_1$ and $\mathcal{G}_2$ separately. The identity of $\mathcal{G}_1 \otimes \mathcal{G}_2$ is (E_1, E_2), as for all $T_1 \in \mathcal{G}_1$ and $T_2 \in \mathcal{G}_2$

$$(T_1, T_2)(E_1, E_2) = (E_1, E_2)(T_1, T_2) = (T_1, T_2).$$

Finally, the inverse of (T_1, T_2) is (T_1^{-1}, T_2^{-1}), which is also a member of $\mathcal{G}_1 \otimes \mathcal{G}_2$.

If $\mathcal{G}_1$ and $\mathcal{G}_2$ are finite groups of orders g_1, and g_2 respectively, then $\mathcal{G}_1 \otimes \mathcal{G}_2$ has order $g_1 g_2$.

The properties of $\mathcal{G}_1 \otimes \mathcal{G}_2$ are best presented in the form of a theorem (all the assertions of which have trivial proofs).

Theorem II

(a) $\mathcal{G}_1 \otimes \mathcal{G}_2$ contains a subgroup consisting of the elements (T_1, E_2), $T_1 \in \mathcal{G}_1$, that is isomorphic to $\mathcal{G}_1$, the isomorphic mapping being $\phi(T_1, E_2) = T_1$.

(b) $\mathcal{G}_1 \otimes \mathcal{G}_2$ contains a subgroup consisting of the elements (E_1, T_2), $T_2 \in \mathcal{G}_2$, that is isomorphic to $\mathcal{G}_2$, the isomorphic mapping being $\psi(E_1, T_2) = T_2$.

(c) The elements of these two subgroups commute with each other, that is

$$(T_1, E_2)(E_1, T_2) = (E_1, T_2)(T_1, E_2) = (T_1, T_2)$$

for all $T_1 \in \mathcal{G}_1$ and $T_2 \in \mathcal{G}_2$.

(d) These two subgroups have only one element in common, namely the identity (E_1, E_2).

(e) Every element of $\mathcal{G}_1 \otimes \mathcal{G}_2$ is the product of an element of the first subgroup with an element of the second subgroup. That is, for all $T_1 \in \mathcal{G}_1$ and $T_2 \in \mathcal{G}_2$,

$$(T_1, T_2) = (T_1, E_2)(E_1, T_2).$$

As isomorphic groups have identical structures, it is natural to now *extend* the definition of a direct product.

Enlarged definition *Direct product group*
A group $\mathcal{G}'$ is said to be a "direct product group" if it is *isomorphic* to a group $\mathcal{G}'_1 \otimes \mathcal{G}'_2$ constructed as in the first theorem above.

With this extension the elements of a direct product group need no longer be in the form of pairs. Such a group can be identified by the following theorem, which is essentially the converse of that immediately above.

Theorem III If a group $\mathcal{G}'$ possesses two subgroups $\mathcal{G}'_1$ and $\mathcal{G}'_2$ such that

(a) the elements of $\mathcal{G}'_1$ commute with the elements of $\mathcal{G}'_2$,

(b) $\mathcal{G}'_1$ and $\mathcal{G}'_2$ have only the identity element in common, and

(c) every element of $\mathcal{G}'$ can be written as a product of an element of $\mathcal{G}'_1$ with an element of $\mathcal{G}'_2$,

then $\mathcal{G}'$ is a direct product group that is isomorphic to $\mathcal{G}'_1 \otimes \mathcal{G}'_2$.

Proof See, for example, Chapter 2, Section 7, of Cornwell (1984).

Example I *The group* O(3) *as a direct product group*
The group O(3) is isomorphic to SO(3) $\otimes \mathcal{G}_2'$, where $\mathcal{G}_2'$ is the matrix group of order 2 consisting of the matrices $\mathbf{1}_3$ and $-\mathbf{1}_3$, as the properties (a), (b) and (c) of the preceding theorem are obviously satisfied.

As O(3) is isomorphic to the group of all rotations in three dimensions, and as SO(3) is isomorphic to the subgroup of proper rotations (see Chapter 1, Section 2), this implies that the group of *all* rotations is isomorphic to the direct product of the group of *proper* rotations and the group $\{E, I\}$ consisting of the identity transformation E and the spatial inversion operator I.

It should be observed that condition (a) of the last theorem can be replaced by an equivalent condition (a'), which reads:

(a) $\mathcal{G}_1'$ and $\mathcal{G}_2'$ are both *invariant* subgroups of $\mathcal{G}'$.

(Obviously (a) implies (a'). Conversely, if (a') is true, then for any $T_1' \in \mathcal{G}_1'$ and $T_2' \in \mathcal{G}_2'$, $T_1'T_2'(T_1')^{-1} = T_2'' \in \mathcal{G}_2'$. Similarly $(T_2')^{-1}T_1'T_2' = T_1'' \in \mathcal{G}_1'$, so that $(T_2')^{-1}T_1'T_2'(T_1')^{-1} = T_1''(T_1')^{-1} = (T_2')^{-1}T_2''$. As $T_1''(T_1')^{-1} \in \mathcal{G}_1'$ and $(T_2')^{-1}T_2'' \in \mathcal{G}_2'$, (b) implies that $T_1' = T_1''$ and $T_2' = T_2''$. Thus $(T_2')^{-1}T_1'T_2' = T_1'$ for all $T_1' \in \mathcal{G}_1'$ and $T_2' \in \mathcal{G}_2'$, so that $\mathcal{G}_1'$ and $\mathcal{G}_2'$ commute.)

The notion of a semi-direct product group $\mathcal{G}'$ is essentially a generalization of that of a direct product group in which conditions (b) and (c) of the last theorem are retained intact but condition (a') is weakened to the requirement that only $\mathcal{G}_1'$ must be an invariant subgroup, but $\mathcal{G}_2'$, although remaining a subgroup of $\mathcal{G}'$, need not be invariant.

Definition *Semi-direct product group*
A group $\mathcal{G}'$ is said to be a "semi-direct product group" if it possesses two subgroups $\mathcal{G}_1'$ and $\mathcal{G}_2'$ such that

(a) $\mathcal{G}_1'$ is an invariant subgroup of $\mathcal{G}'$;

(b) $\mathcal{G}_1'$ and $\mathcal{G}_2'$ have only the identity element in common; and

(c) every element of $\mathcal{G}'$ can be written as a product of an element of $\mathcal{G}_1'$ with an element of $\mathcal{G}_2'$.

$\mathcal{G}'$ may then be said to be isomorphic to $\mathcal{G}_1' \circledS \mathcal{G}_2'$.

As in the special case of a direct product group, the requirement (b) always implies that the decomposition (c) is unique.

Example II *The Euclidean group of* $\mathbb{R}^3$ *as a semi-direct product group*
The Euclidean group $\mathcal{G}'$ of $\mathbb{R}^3$ is defined to be the group of all linear coordinate transformations T, with Equation (1.7) giving the group multiplication operation. Let $\mathcal{G}_1'$ be the subgroup of pure translations and $\mathcal{G}_2'$ the subgroup of pure rotations. Then for any $T_1 \in \mathcal{G}_1'$ and any $T \in \mathcal{G}'$, from Equations (1.7) and (1.8),

$$\{\mathbf{R}(T)|\mathbf{t}(T)\}\{\mathbf{1} \mid \mathbf{t}(T_1)\}\{\mathbf{R}(T)|\mathbf{t}(T)\}^{-1} = \{\mathbf{1} \mid \mathbf{R}(T)\mathbf{t}(T_1)\},$$

so that $\mathcal{G}_1'$ is an invariant subgroup of $\mathcal{G}'$. Moreover, for any $T \in \mathcal{G}'$,

$$\{\mathbf{R}(T)|\mathbf{t}(T)\} = \{\mathbf{1} \mid \mathbf{t}(T)\}\{\mathbf{R}(T) \mid \mathbf{0}\},$$

so that requirement (c) is also satisfied, while (b) is obvious. Thus $\mathcal{G}'$ is isomorphic to $\mathcal{G}_1' \circledS \mathcal{G}_2'$.

A further important set of examples is provided by the symmorphic crystallographic space groups. These will be discussed in detail in Chapter 7.

Although it is possible to give an abstract construction of a semidirect product of certain groups in terms of pairs of elements from the two groups, the procedure is much more elaborate than for the direct product (Lomont 1959, page 29). Fortunately, all the physically important examples of groups having a semi-direct product structure occur naturally, so this abstract construction will be omitted here.

Chapter 3

Lie Groups

It is now time to formulate a definition of a Lie group and to describe some of the major properties of such groups. Readers whose interests lie only in the applications to solid state physics (where only finite groups appear) may safely omit this chapter.

1 Definition of a linear Lie group

A Lie group embodies three different forms of mathematical structure. Firstly, it satisfies the group axioms of Chapter 1 and so has the group structure described in Chapter 2. Secondly, the elements of the group also form a "topological space", so that it may be described as being a special case of a "topological group". Finally, the elements also constitute an "analytic manifold". Consequently a Lie group can be defined in several different (but equivalent) ways, depending on the degree of emphasis that is being accorded to the various aspects. In particular, it can be defined as a topological group with certain additional analytic properties (Pontrjagin 1946, 1986) or, alternatively, as an analytic manifold with additional group properties (Chevalley 1946, Adams 1969, Varadarajan 1974, Warner 1971). Both of these formulations involve the introduction of a series of ancillary concepts of a rather abstract nature.

Very fortunately, every Lie group that is important in physical problems is of a type, known as a "linear Lie group", for which a relatively straightforward definition can be given. As will be seen, this definition is both precise and simple, in that it involves only familiar concrete objects such as matrices and contains no mention of topological spaces or analytic manifolds. (Readers who are interested in the *general* definition of a Lie group in terms of analytic manifolds may, for example, find this formulation in Appendix J of Cornwell (1984).)

The basic feature of any Lie group is that it has a non-countable number of elements lying in a region "near" its identity and that the structure of this region both very largely determines the structure of the whole group and

is itself determined by its corresponding real Lie algebra. To ensure that this is so, the elements in this region must be parametrized in a particular analytic way. Of course, to say that certain elements are "near" the identity means that a notion of "distance" has to be composed, and it is here that the complications of the general treatment start. However, all the Lie groups of physical interest are "linear", in the sense that they have at least one faithful finite-dimensional representation. This representation can be used to provide the necessary precise formulation of distance and to ensure that all the other topological requirements are automatically observed.

Definition *Linear Lie group of dimension n*
A group $\mathcal{G}$ is a linear Lie group of dimension n if it satisfies the following conditions (A), (B), (C) and (D):

(A) *$\mathcal{G}$ must possess at least one faithful finite-dimensional representation* $\mathbf{\Gamma}$.

Suppose that this representation has dimension m. Then the "distance" $d(T,T')$ between two elements T and T' of $\mathcal{G}$ may be *defined* by

$$d(T,T') = +\{\sum_{j=1}^{m}\sum_{k=1}^{m} |\, \Gamma(T)_{jk} - \Gamma(T')_{jk} \,|^2\}^{1/2}. \tag{3.1}$$

(This distance function $d(T,T')$ will be called the "metric".) Then

(i) $d(T',T) = d(T,T')$;

(ii) $d(T,T) = O$;

(iii) $d(T,T') > O$ if $T \neq T'$;

(iv) if T, T' and T'' are any three elements of $\mathcal{G}$,

$$d(T,T'') \leq d(T,T') + d(T',T''),$$

all of which are essential for the interpretation of $d(T,T')$ as a distance. (The choice of this metric implies that the group is being endowed with the topology of the m^2-dimensional complex Euclidean space $\mathbb{C}^{m^2}$ (see Example II of Appendix B, Section 2).) The set of elements T of $\mathcal{G}$ such that

$$d(T,E) < \delta,$$

where δ is positive real number, is then said to "lie in a sphere of radius δ centred on the identity E", which will be denoted by M_δ. Such a sphere will be sometimes referred to as a "small neighbourhood" of E.

(B) *There must exist a $\delta > 0$ such that every element T of $\mathcal{G}$ lying in the sphere M_δ of radius δ centred on the identity can be parametrized by n real parameters $x_1, x_2, \ldots, x_n$ (no two such sets of parameters corresponding to the same element T of $\mathcal{G}$), the identity E being parametrized by $x_1 = x_2 = \ldots = x_n = 0$.*

Thus every element of M_δ corresponds to one and only one point in an n-dimensional real Euclidean space $\mathbb{R}^n$, the identity E corresponding to the origin $(0,0,\ldots,0)$ of $\mathbb{R}^n$. Moreover, no point in $\mathbb{R}^n$ corresponds to more than one element T in M_δ.

(C) *There must exist a* $\eta > 0$ *such that every point in* $\mathbb{R}^n$ *for which*

$$\sum_{j=1}^{n} x_j^2 < \eta^2 \tag{3.2}$$

corresponds to some element T *in* M_δ.

The set of point elements T so obtained will be denoted by R_η. Thus R_η is a subset of M_δ, and there is a *one-to-one* correspondence between elements of $\mathcal{G}$ in R_η, and points in $\mathbb{R}^n$ satisfying Condition (3.2).

The final set of conditions ensures that in terms of this parametrization the group multiplication operation is expressible in terms of analytic functions. Let $T(x_1, x_2, \ldots, x_n)$ denote the element of $\mathcal{G}$ corresponding to a point satisfying Condition (3.2) and define $\mathbf{\Gamma}(x_1, x_2, \ldots, x_n)$ by $\mathbf{\Gamma}(x_1, x_2, \ldots, x_n) = \mathbf{\Gamma}(T(x_1, x_2, \ldots, x_n))$ for all $(x_1, x_2, \ldots, x_n)$ satisfying Condition (3.2).

(D) *Each of the matrix elements of* $\mathbf{\Gamma}(x_1, x_2, \ldots, x_n)$ *must be an analytic function of* $x_1, x_2, \ldots, x_n$ *for all* $(x_1, x_2, \ldots, x_n)$ *satisfying Condition (3.2).*

The term "analytic" here means that each of the matrix elements Γ_{jk} must be expressible as a power series in $x_1 - x_1^0, x_2 - x_2^0, \ldots, x_n - x_n^0$ for all $(x_1^0, x_2^0, \ldots, x_n^0)$ satisfying Condition (3.2). This implies that *all* the derivatives $\partial\Gamma_{jk}/\partial x^p$, $\partial^2\Gamma_{jk}/\partial x^p \partial x^q$ etc. must exist for all $j,k = 1,2,\ldots,m$ at all points satisfying Condition (3.2), including in particular the point (0,0,...,0) (Fleming 1977). In particular one can *define* the n $m \times m$ matrices $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n$ by

$$(\mathbf{a}_p)_{jk} = (\partial\Gamma_{jk}/\partial x^p)_{x_1=x_2=\ldots=x_n=0} \,. \tag{3.3}$$

These conditions together imply the following very important theorem.

Theorem I The matrices $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n$ defined by Equation (3.3) form the basis for a n-dimensional *real* vector space.

Proof See, for example, Chapter 3, Section 1, of Cornwell (1984).

It should be noted that, although $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n$ form the basis of a *real* vector space, there is no requirement that the matrix elements of these matrices need be real. (This point is demonstrated explicitly in Example III.)

It will be shown in Chapter 8 that the matrices $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n$ actually form the basis of a "real Lie algebra", a vital observation on which most of the subsequent theory is founded. However, the rest of the present chapter will be devoted to "group theoretical" aspects of linear Lie groups.

The above definition requires a parametrization only of the group elements belonging to a small neighbourhood of the identity element. In some cases this parametrization by a single set of n parameters $x_1, x_2, \ldots, x_n$ is valid over a large part of the group or even over the whole group, but this is not essential. In Section 2 it will be shown that the whole of the "connected" subgroup of a linear Lie group of dimension n can be given a parametrization in terms of a single set of n real numbers which will be denoted by $y_1, y_2, \ldots, y_n$. However, this latter parametrization is not required to satisfy all the conditions of the above definition, and so need bear little relation to the parametrization by $x_1, x_2, \ldots, x_n$.

The following examples have been chosen because they illustrate all the essential points of the definition without involving any heavy algebra.

Example I *The multiplicative group of real numbers*
As in Example I of Chapter 1, Section 1, let $\mathcal{G}$ be the group of real numbers t ($t \neq 0$) with ordinary multiplication as the group multiplication operation, the identity E being the number 1. $\mathcal{G}$ has the obvious one-dimensional faithful representation $\mathbf{\Gamma}(t) = [t]$, so condition (A) is satisfied and the metric d of Equation (3.1) is given by $d(t, t') = |t - t'|$. In particular, $d(t, 1) = |t - 1|$. Let $\delta = \frac{1}{2}$ so that $\frac{1}{2} < t < 2$ for all t in M_δ. A convenient parametrization for $t \in M_\delta$ is then

$$t = \exp x_1. \tag{3.4}$$

As required in (B), the identity 1 corresponds to $x_1 = 0$. Condition (C) is obeyed with $\eta = \log \frac{3}{2}$, as $x_1^2 < (\log \frac{3}{2})^2$ implies $\frac{2}{3} < \exp x_1 < \frac{3}{2}$. By Equation (3.4) $\Gamma(x_1) = \exp x_1$, which is certainly analytic, so that condition (D) is satisfied. Thus $\mathcal{G}$ is a linear Lie group of dimension 1. It should be noted that Equation (3.3) implies that $\mathbf{a}_1 = [1]$, thereby confirming the first theorem above.

It is significant that the parametrization in Equation (3.4) extends to *all* $t > 0$ (with $-\infty < x_1 < +\infty$) and that this set forms a subgroup of $\mathcal{G}$. Moreover, every group element t such that $t < 0$ can be written in the form $t = (-1) \exp x_1$ for some x_1.

Example II *The groups* O(2) *and* SO(2)
O(2) is the group of all real orthogonal 2×2 matrices $\mathbf{A}$, SO(2) being the subgroup for which $\det \mathbf{A} = +1$.

If $\mathbf{A} \in \mathrm{O}(2)$, $\mathbf{\Gamma}(\mathbf{A}) = \mathbf{A}$ provides a faithful finite-dimensional representation. The orthogonality conditions $\tilde{\mathbf{A}}\mathbf{A} = \mathbf{A}\tilde{\mathbf{A}} = \mathbf{1}$ require that

$$\begin{aligned} (A_{11})^2 + (A_{12})^2 &= (A_{11})^2 + (A_{21})^2 = (A_{21})^2 + (A_{22})^2 \\ &= (A_{12})^2 + (A_{22})^2 = 1 \end{aligned} \tag{3.5}$$

and

$$A_{11}A_{21} + A_{22}A_{12} = A_{11}A_{12} + A_{22}A_{21} = 0. \tag{3.6}$$

Equations (3.5) imply that $(A_{11})^2 = (A_{22})^2$ and $(A_{12})^2 = (A_{21})^2$, so that there are only two sets of solutions of Equations (3.6), namely:

(i) $A_{11} = A_{22}$ and $A_{12} = -A_{21}$. Equations (3.5) imply that $\det \mathbf{A} = +1$, i.e. $\mathbf{A} \in \mathrm{SO}(2)$. Moreover, from Equations (3.5), $d(\mathbf{A}, \mathbf{1}) = 2(1 - A_{11})^{1/2}$.

(ii) $A_{11} = -A_{22}$ and $A_{12} = A_{21}$. In this case $\det \mathbf{A} = -1$ and $d(\mathbf{A}, \mathbf{1}) = 2$.

With the choice $\delta = \sqrt{2}$, condition (B) requires the parametrization of part of set (i) but it is not necessary to include set (ii), as it is completely outside M_δ. A convenient parametrization is

$$\mathbf{A} = \mathbf{\Gamma}(\mathbf{A}) = \begin{bmatrix} \cos x_1 & \sin x_1 \\ -\sin x_1 & \cos x_1 \end{bmatrix}. \tag{3.7}$$

Clearly $x_1 = 0$ corresponds to the group identity $\mathbf{1}$ and the dimension n is 1.

Every point of $\mathbb{R}^1$ such that $x_1^2 < (\pi/3)^2$ gives a matrix $\mathbf{A}$ in M_δ, so condition (C) is satisfied. In fact the parametrization of Equation (3.7) extends to the whole of the set (i) with $-\pi \leq x_1 \leq \pi$, that is, to the whole of SO(2). Condition (D) is obviously obeyed, so O(2) and SO(2) are both linear Lie groups of dimension 1. Further, Equation (3.3) gives

$$\mathbf{a}_1 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix},$$

again confirming the first theorem above.

Although the parametrization of Equation (3.7) extends to the whole of SO(2), it cannot apply to the set (ii). However, every $\mathbf{A}$ of set (ii) can be written as

$$\mathbf{A} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} \cos x_1 & \sin x_1 \\ -\sin x_1 & \cos x_1 \end{bmatrix} = \begin{bmatrix} -\sin x_1 & \cos x_1 \\ \cos x_1 & \sin x_1 \end{bmatrix} \tag{3.8}$$

for some x_1 such that $-\pi \leq x_1 \leq \pi$.

Example III *The group* SU(2)

SU(2) is the group of 2×2 unitary matrices $\mathbf{u}$ with $\det \mathbf{u} = 1$. A faithful finite-dimensional representation is provided by $\mathbf{\Gamma}(\mathbf{u}) = \mathbf{u}$. The defining conditions imply that every $\mathbf{u} \in \mathrm{SU}(2)$ has the form

$$\mathbf{u} = \begin{bmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{bmatrix}, \tag{3.9}$$

where α and β are two complex numbers such that $|\alpha|^2 + |\beta|^2 = 1$. With $\alpha = \alpha_1 + i\alpha_2$, $\beta = \beta_1 + i\beta_2$ ($\alpha_1, \alpha_2, \beta_1, \beta_2$ being real), this latter condition becomes $\alpha_1^2 + \alpha_2^2 + \beta_1^2 + \beta_2^2 = 1$. An appropriate parametrization is then

$$\alpha_2 = x_3/2,\ \beta_1 = x_2/2,\ \beta_2 = x_1/2,\ \alpha_1 = +\{1 - (1/4)(x_1^2 + x_2^2 + x_3^2)\}^{1/2},$$

for then $x_1 = x_2 = x_3 = 0$ corresponds to the identity $\mathbf{1}$, and

$$d(\mathbf{u}, \mathbf{1}) = 2[1 - \{1 - (1/4)(x_1^2 + x_2^2 + x_3^2)\}^{1/2}]^{1/2},$$

so that $d(\mathbf{u}, \mathbf{1}) < \delta$ if and only if $x_1^2 + x_2^2 + x_3^2 < \{2\delta^2 - \frac{1}{4}\delta^4\}^{1/2}$. Thus, with $\delta < 2\sqrt{2}$ and $\eta < 2\delta^2 - \frac{1}{4}\delta^4$, conditions (B) and (C) are satisfied and M_δ and R_η coincide. Condition (D) is clearly true, so SU(2) is a linear Lie group of dimension 3. Incidentally, Equation (3.3) gives

$$\mathbf{a}_1 = \frac{1}{2}\begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix}, \mathbf{a}_2 = \frac{1}{2}\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \mathbf{a}_3 = \frac{1}{2}\begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}, \tag{3.10}$$

so that the first theorem above is yet again confirmed.

Although this parametrization is the most convenient for establishing that SU(2) is a linear Lie group, it is not the most useful for some practical calculations. Indeed only the matrices $\mathbf{u}$ with $\alpha_1 \geq 0$ can be parametrized this way, whereas it will be shown in Example III of Section 2 that there exist parametrizations of the whole of SU(2).

There is no difficulty in principle in generalizing the arguments used in Examples II and III to show that for all $N \geq 2$, O(N), SO(N), U(N) and SU(N) are linear Lie groups of dimensions $\frac{1}{2}N(N-1)$, $\frac{1}{2}N(N-1)$, N^2 and $N^2 - 1$ respectively, but the detailed algebra is rather more lengthy. (U(1) is a special case that is very easy to treat along the lines of Example I, because $\mathbf{u} = [\exp ix_1]$, $-\pi \leq x_1 \leq \pi$, is a parametrization.)

Finally, a Lie subgroup can be defined in the obvious way.

Definition *Lie subgroup of a linear Lie group*
A subgroup $\mathcal{G}'$ of a linear Lie group $\mathcal{G}$ that is itself a linear Lie group is called a "Lie subgroup" of $\mathcal{G}$.

2 The connected components of a linear Lie group

Definition *Connected component of a linear Lie group $\mathcal{G}$*
A maximal set of elements T of $\mathcal{G}$ that can be obtained from each other by continuously varying one or more of the matrix elements $\Gamma(T)_{jk}$ of the faithful finite-dimensional representation $\mathbf{\Gamma}$ is said to form a "connected component" of $\mathcal{G}$.

(It can be shown that the concept of connectedness as defined for a general topological space (Simmons 1963) is equivalent, for the type of space being considered here, to that implied by the above definition.)

Example I *The multiplicative group of real numbers*
This group was considered in Example I of Section 1. The set $t > 0$ forms

one connected component (which actually constitutes a subgroup) and the set $t < 0$ forms another connected component. As $t = 0$ is excluded from the group, one set cannot be obtained continuously from the other.

Example II *The groups* O(2) *and* SO(2)
In the group O(2) that was examined in Example II of Section 1, every matrix $\mathbf{A}$ of SO(2) can be parametrized by Equation (3.7) with $-\pi \leq x_1 \leq \pi$, whereas if $\mathbf{A}$ is a member of the set (ii) (i.e. if $\det \mathbf{A} = -1$), $\mathbf{A}$ can be written in the form of Equation (3.8). Thus SO(2) constitutes one connected component and the set (ii) is another connected component. It is obvious that these two sets cannot be connected to each other, because in a connected component $\det \mathbf{\Gamma}(T)$ must vary continuously with T (if it varies at all), but $\det \mathbf{A}$ cannot take any values between $+1$ and -1 for $\mathbf{A} \in$ O(2).

These examples suggest the following general theorem.

Theorem I The connected component of a linear Lie group $\mathcal{G}$ that contains the identity E is an *invariant subgroup* of $\mathcal{G}$. This component is often referred to as "the connected subgroup of $\mathcal{G}$". Moreover, each connected component of a linear Lie group $\mathcal{G}$ is a right coset of the connected subgroup.

Proof See, for example, Chapter 3, Section 2, of Cornwell (1984).

In principle $\mathcal{G}$ may have a countably infinite number of connected components, but in all cases of physical interest this number is finite. The axioms imply that the connected subgroup is always a linear Lie group.

Definition *Connected linear Lie group*
A linear Lie group is said to be "connected" if it possesses *only one* connected component.

Thus the whole of a connected linear Lie group of dimension n can be parametrized by n real numbers $y_1, y_2, \ldots, y_n$ which form a connected set in $\mathbb{R}^n$ in such a way that all the matrix elements $\Gamma(T)_{jk}$ are *continuous* functions of the parameters. There is no requirement that these functions be analytic nor that they provide a one-to-one mapping. Consequently this parametrization does not necessarily satisfy all the conditions appearing in the definition of a linear Lie group. As the sets $x_1, x_2, \ldots, x_n$ and $y_1, y_2, \ldots, y_n$ are required for different purposes, they need not be interchangeable. The parametrizations do coincide in Examples I and II above, but Example III below reflects the general situation.

Example III *The group* SU(2)
Every pair of complex numbers α and β of Equation (3.9) that satisfy the condition $|\alpha|^2 + |\beta|^2 = 1$ can be written as

$$\alpha = \cos y_1 \exp(iy_2), \ \beta = \sin y_1 \exp(iy_3),$$

where

$$0 \leq y_1 \leq \pi/2,\ 0 \leq y_2 \leq 2\pi,\ 0 \leq y_3 \leq 2\pi. \tag{3.11}$$

Thus

$$\mathbf{u} = \mathbf{\Gamma}(\mathbf{u}) = \begin{bmatrix} \cos y_1 \exp(iy_2) & \sin y_1 \exp(iy_3) \\ -\sin y_1 \exp(-iy_3) & \cos y_1 \exp(-iy_2) \end{bmatrix}, \tag{3.12}$$

whose matrix elements are obviously continuous functions of y_1, y_2 and y_3. This is therefore a parametrization of the whole of SU(2). (This parametrization fails to satisfy the conditions involved in the definition of a linear Lie group because it does not provide a *one-to-one* mapping of the appropriate regions, for the identity corresponds to the whole set of points $y_1 = 0$, $y_2 = 0$, $0 \leq y_3 \leq 2\pi$. Consequently $\partial\mathbf{\Gamma}/\partial y_3 = \mathbf{0}$ at $y_1 = y_2 = y_3 = 0$.)

Similar arguments show that SO(N) and SU(N) are connected linear Lie groups for all $N \geq 2$, as is U(N) for all $N \geq 1$. The relationship between a connected linear Lie group and its corresponding real Lie algebra will be studied in some detail in Chapter 8, where it will be shown that the Lie algebra very largely determines the structure of the group. Indeed, it is for this purpose that the parametrization in terms of $x_1, x_2, \ldots, x_n$ is required. However, the rest of this chapter is devoted to certain "global" properties of linear Lie groups, and for these it is the parametrization in terms of $y_1, y_2, \ldots, y_n$ that is relevant.

3 The concept of compactness for linear Lie groups

Although the concept of a "compact" set in a general topological space has a curiously elusive quality, the following theorem, often referred to as the "Heine-Borel Theorem", provides a very straightforward characterization of such sets in finite-dimensional real and complex Euclidean spaces. As this will suffice to distinguish a compact linear Lie group from a non-compact linear Lie group, no attempt will be made to give a detailed account of compactness, nor even a definition of the notion. (A lucid account of this and other general topological ideas may be found in the book of Simmons (1963).)

Theorem I A subset of points of a real or complex finite-dimensional Euclidean space is "compact" if and only if it is *closed* and *bounded*.

As mentioned in Section 1, by introducing the faithful m-dimensional representation $\mathbf{\Gamma}$, the Lie group has been endowed with the topology of $\mathbb{C}^{m^2}$. However, it is often helpful to invoke the continuous parametrization of the connected subgroup by $y_1, y_2, \ldots, y_n$ introduced in Section 2. As the continuous image of a compact set is always another compact set (Simmons 1963), it

follows that if the linear Lie group has only a finite number of connected components and the parameters $y_1, y_2, \ldots, y_n$ range over a closed and bounded set in $\mathbb{R}^n$, then the group is compact.

A "bounded" set of a real or complex Euclidean space is merely a set that can be contained in a *finite* "sphere" of the space. The term "closed" implies something more involved, so perhaps a few words of explanation may be needed. Although the specification of a general closed set can be fairly difficult, the only subsets of $\mathbb{R}^n$ that are relevant here are connected, and for these the characterization is straightforward. Indeed, in $\mathbb{R}^1$ every connected closed set is of the form $a_1 \leq y_1 \leq b_1$. Similarly, the set $a_j \leq y_j \leq b_j$, $j = 1, 2, \ldots, n$, of $\mathbb{R}^n$ is closed, but if any of the end points a_j and b_j are not attained the set is not closed. This set is bounded if and only if all the a_j and b_j are finite.

These considerations imply the following identification.

Characterization *Compact linear Lie group of dimension n*
A linear Lie group of dimension n with a finite number of connected components is *compact* if the parameters $y_1, y_2, \ldots, y_n$ range over the closed finite intervals $a_j \leq y_j \leq b_j$, $j = 1, 2, \ldots, n$.

The Lie groups of physical interest that are non-compact usually fail to be compact by virtue of giving an unbounded set of matrix elements in $\mathbb{C}^{m^2}$. As the sets of matrix elements $\Gamma(T)_{jk}$ of a linear Lie group $\mathcal{G}$ are bounded if and only if there exists a finite real number M such that $d(T, E) < M$ for all $T \in \mathcal{G}$, such groups are very easy to recognize in practice.

If a Lie group $\mathcal{G}$ is compact, then every Lie subgroup $\mathcal{S}$ of $\mathcal{G}$ must also be compact (except in the rare case when $\mathcal{S}$ has a "non-closed" parametrization). On the other hand, if $\mathcal{G}$ is non-compact, $\mathcal{S}$ may easily possess compact Lie subgroups.

For semi-simple Lie groups there exists a criterion for compactness that is expressed purely in Lie algebraic terms, as will be shown in Chapter 11, Section 10.

The real importance of the distinction between compact and non-compact groups lies in the fact that the representation theory of compact Lie groups is very largely the same as that for finite groups, whereas for non-compact groups the theory is entirely different.

Example I *The multiplicative group of real numbers*
As noted in Example I of Section 1, a faithful one-dimensional representation of this group is provided by $\mathbf{\Gamma}(t) = [t]$. Obviously this set is unbounded in $\mathbb{C}^1$, so the group is *non-compact.*

Example II *The groups* $\mathrm{O}(N)$ *and* $\mathrm{SO}(N)$
For O(2) and SO(2), Examples II of Sections 1 and 2 imply that the range of the only parameter $y_1 (= x_1)$ is $-\pi \leq y_1 \leq \pi$. Similar statements are true for $\mathrm{O}(N)$ and $\mathrm{SO}(N)$ for $N \geq 3$, and consequently $\mathrm{O}(N)$ and $\mathrm{SO}(N)$ are *compact*

for all $N \geq 2$.

Example III *The groups* $\mathrm{U}(N)$ *and* $\mathrm{SU}(N)$
As all the intervals in Conditions (3.11) are closed and finite, $\mathrm{SU}(2)$ is *compact.* The same is true of $\mathrm{SU}(N)$ for all $N \geq 2$, and of $\mathrm{U}(N)$ for all $N \geq 1$.

4 Invariant integration

If to each element T of a group $\mathcal{G}$ a complex number $f(T)$ is assigned, then $f(T)$ is said to be a "complex-valued function defined on $\mathcal{G}$". One example that has been met already is the set of matrix elements $\Gamma(T)_{jk}$ (for j, k fixed) of a matrix representation $\mathbf{\Gamma}$ of $\mathcal{G}$.

For a *finite* group sums of the form $\sum_{T\in\mathcal{G}} f(T)$ are frequently encountered, particularly in representation theory. Because the Rearrangement Theorem shows that the set $\{T'T; T \in \mathcal{G}\}$ has exactly the same members as $\mathcal{G}$, it follows that for any $T' \in \mathcal{G}$

$$\sum_{T\in\mathcal{G}} f(T'T) = \sum_{T\in\mathcal{G}} f(T),$$

and the sum is said to be "left-invariant". Similarly

$$\sum_{T\in\mathcal{G}} f(TT') = \sum_{T\in\mathcal{G}} f(T),$$

so such sums are also "right-invariant". Moreover, with $f(T) = 1$ for all $T \in \mathcal{G}$, the sum is finite in the sense that $\sum_{T\in\mathcal{G}} 1 = g$, the order of $\mathcal{G}$.

In generalizing to a connected linear Lie group, it is natural to make the hypothesis that the sum can be replaced by an integral with respect to the parameters $y_1, y_2, \ldots, y_n$. However, questions immediately arise about the left-invariance, right-invariance and finiteness of such integrals. For general topological groups these become problems in measure theory. Using this theory Haar (1933) showed that for a very large class of topological groups, which includes the linear Lie groups, there always exists a left-invariant integral and there always exists a right-invariant integral. (Accounts of these developments, including proofs of the theorems that follow, may be found in the books of Halmos (1950), Loomis (1953) and Hewitt and Ross (1963).)

Let

$$\int_{\mathcal{G}} f(T)\, d_l T \equiv \int_{a_1}^{b_1} dy_1 \ldots \int_{a_n}^{b_n} dy_n\, f(T(y_1, \ldots, y_n))\sigma_l(y_1, \ldots, y_n) \qquad (3.13)$$

and

$$\int_{\mathcal{G}} f(T)\, d_r T \equiv \int_{a_1}^{b_1} dy_1 \ldots \int_{a_n}^{b_n} dy_n\, f(T(y_1, \ldots, y_n))\sigma_r(y_1, \ldots, y_n) \qquad (3.14)$$

be the left- and right-invariant integrals of a linear Lie group $\mathcal{G}$, so that

$$\int_{\mathcal{G}} f(T'T)\, d_l T = \int_{\mathcal{G}} f(T)\, d_l T \qquad (3.15)$$

$$\int_{\mathcal{G}} f(TT')\, d_r T = \int_{\mathcal{G}} f(T)\, d_r T \tag{3.16}$$

for any $T' \in \mathcal{G}$ and any function $f(T)$ for which the integrals are well defined. Here $\sigma_l(y_1, \ldots, y_n)$ and $\sigma_r(y_1, \ldots, y_n)$ are left- and right-invariant "weight functions", which are each unique up to multiplication by arbitrary constants. The left- and right-invariant integrals may be said to be *finite* if

$$\int_{\mathcal{G}} d_l T \equiv \int_{a_1}^{b_1} dy_1 \ldots \int_{a_n}^{b_n} dy_n\, \sigma_l(y_1, \ldots, y_n)$$

and

$$\int_{\mathcal{G}} d_r T \equiv \int_{a_1}^{b_1} dy_1 \ldots \int_{a_n}^{b_n} dy_n\, \sigma_r(y_1, \ldots, y_n)$$

are finite. If the multiplicative constants can be chosen so that $\sigma_l(y_1, \ldots, y_n)$ and $\sigma_r(y_1, \ldots, y_n)$ are equal, so that the integrals are both left- and right-invariant, then $\mathcal{G}$ is said to be "unimodular", and one may write

$$d_l T = d_r T = dT$$

and

$$\sigma_l(y_1, \ldots, y_n) = \sigma_r(y_1, \ldots, y_n) = \sigma(y_1, \ldots, y_n).$$

If $\mathcal{G}$ has more than one connected component, the integrals in Equations (3.13) and (3.14) can be generalized in the obvious way to include a sum over the components.

The significance of the distinction between compact and non-compact Lie groups lies in the first two of the following theorems, the first of which was originally proved by Peter and Weyl (1927). They imply that compact Lie groups have many of the properties of finite groups, summation over a finite group merely being replaced by an invariant integral over the compact Lie groups, whereas for non-compact groups the situation is completely different.

Theorem I If $\mathcal{G}$ is a *compact* Lie group, then $\mathcal{G}$ is *unimodular* and the invariant integral

$$\int_{\mathcal{G}} f(T)\, dT \equiv \int_{a_1}^{b_1} dy_1 \ldots \int_{a_n}^{b_n} dy_n\, f(T(y_1, \ldots, y_n))\sigma(y_1, \ldots, y_n)$$

exists and is *finite* for every continuous function $f(T)$. Thus $\sigma(y_1, \ldots, y_n)$ can be chosen so that

$$\int_{\mathcal{G}} dT \equiv \int_{a_1}^{b_1} dy_1 \ldots \int_{a_n}^{b_n} dy_n\, \sigma(y_1, \ldots, y_n) = 1.$$

(A function $f(T)$ is continuous if and only if $f(T(y_1, \ldots, y_n))$ is a continuous function of $y_1, \ldots, y_n$.)

Theorem II If $\mathcal{G}$ is a *non-compact* Lie group then the left- and right-invariant integrals are *both infinite*.

For non-compact groups the question of when $\mathcal{G}$ is unimodular is partially answered by the following theorem.

Theorem III If $\mathcal{G}$ is Abelian or semi-simple then $\mathcal{G}$ is unimodular.

The definition of a semi-simple Lie group is given in Chapter 11, Section 2. The other non-compact linear Lie groups have to be investigated individually. In practice, explicit expressions for weight functions are seldom needed. Indeed, in dealing with the compact Lie groups all that is usually required is the knowledge (embodied in the first theorem above) that finite left- and right-invariant integrals always exist.

Chapter 4

Representations of Groups - Principal Ideas

1 Definitions

The concept of the representation of a group was introduced in Chapter 1, Section 4, where it was shown that representations occur in a natural and significant way in quantum mechanics. It is worth while starting the detailed study of representations by repeating the definition as rephrased in Chapter 2, Section 6:

Definition *Representation of a group* $\mathcal{G}$
If there exists a homomorphic mapping of a group $\mathcal{G}$ onto a group of non-singular $d \times d$ matrices $\mathbf{\Gamma}(T)$, with matrix multiplication as the group multiplication operation, then the group of matrices $\mathbf{\Gamma}(T)$ forms a d-dimensional representation $\mathbf{\Gamma}$ of $\mathcal{G}$.

It will be recalled that the representation is described as being "faithful" if the mapping is one-to-one.

Theorem I If $\mathbf{\Gamma}$ is a d-dimensional representation of a group $\mathcal{G}$, and E is the identity of $\mathcal{G}$, then $\mathbf{\Gamma}(E) = \mathbf{1}_d$.

Proof As $E^2 = E$ then $\mathbf{\Gamma}(E)\{\mathbf{\Gamma}(E) - \mathbf{1}\} = \mathbf{0}$. Suppose first that this is the minimal equation for $\mathbf{\Gamma}(E)$ (see Appendix A, Section 2). This implies that $\mathbf{\Gamma}(E)$ is diagonalizable and has at least one eigenvalue equal to zero, which in turn implies that $\det \mathbf{\Gamma}(E) = 0$. As this is not permitted, the minimal equation must be of degree less than two and so must be of the form $\mathbf{\Gamma}(E) - \gamma\mathbf{1} = \mathbf{0}$, and clearly the only allowed value of γ is 1.

It follows that $\mathbf{\Gamma}(T^{-1}) = \mathbf{\Gamma}(T)^{-1}$ for all $T \in \mathcal{G}$. Every group $\mathcal{G}$ possesses an "identity" representation, which is a one-dimensional representation for

which $\mathbf{\Gamma}(T) = [1]$ for all $T \in \mathcal{G}$. Although mathematically extremely trivial, physically this representation can be very important.

Example I *Some representations of the crystallographic point group* D_4
Several representations of the group D_4 have already been encountered either explicitly or implicitly, and it is worth while gathering them together for future reference. As the subsequent developments will show, this list is far from being exhaustive.

(i) Equation (1.4) implies that the matrices $\mathbf{\Gamma}(T)$ listed in Example III of Chapter 1, Section 2, form a faithful three-dimensional representation of D_4.

(ii) A faithful two-dimensional representation of D_4 was explicitly noted in Example I of Chapter 1, Section 4.

(iii) A non-faithful but non-trivial one-dimensional representation of D_4 is given implicitly in Example I of Chapter 2, Section 6. In this representation

$$\mathbf{\Gamma}(E) = \mathbf{\Gamma}(C_{2y}) = \mathbf{\Gamma}(C_{2x}) = \mathbf{\Gamma}(C_{2z}) = [1],$$
$$\mathbf{\Gamma}(C_{4y}) = \mathbf{\Gamma}(C_{4y}^{-1}) = \mathbf{\Gamma}(C_{2c}) = \mathbf{\Gamma}(C_{2d}) = [-1].$$

(iv) Finally there is the identity representation for which $\mathbf{\Gamma}(T) = [1]$ for all $T \in \mathcal{G}$.

For a Lie group it is necessary to supplement the definition by the requirement that the homomorphic mapping must be *continuous*. For a connected linear Lie group this implies that the matrix elements of the representation must be continuous functions of the parameters $y_1, y_2, \ldots, y_n$ of Chapter 2, Section 2. (The extension to *analytic* representations and the relationship between the two concepts will be considered in Chapter 9, Section 4.)

For groups of coordinate transformations in three-dimensional Euclidean space $\mathbb{R}^3$ it has already been demonstrated how useful are the operators $P(T)$ and the basis functions $\psi_n(\mathbf{r})$ that were defined in Chapter 1, Sections 2 and 4 respectively. It is profitable to partially generalize these concepts to make them available for *any* group $\mathcal{G}$. To this end, consider a d-dimensional representation $\mathbf{\Gamma}$ of $\mathcal{G}$, let $\psi_1, \psi_2, \ldots, \psi_d$ be the basis of a d-dimensional abstract complex inner product space (see Appendix B, Section 2) called the "carrier space" V, and for each $T \in \mathcal{G}$ *define* the operator $\Phi(T)$ acting on the basis by

$$\Phi(T)\psi_n = \sum_{m=1}^{d} \Gamma(T)_{mn}\psi_m, \tag{4.1}$$

for $n = 1, 2, \ldots, d$. With the further definition that

$$\Phi(T)\sum_{j=1}^{d}\{b_j\psi_j\} = \sum_{j=1}^{d} b_j\{\Phi(T)\psi_j\} \tag{4.2}$$

for any set of complex numbers $b_1, b_2, \ldots, b_d$, such an operator is a linear operator. Moreover, Equation (4.1) implies the operator equalities

$$\Phi(T_1T_2) = \Phi(T_1)\Phi(T_2) \tag{4.3}$$

for all $T_1, T_2 \in \mathcal{G}$, so that the operators form a group and there is a homomorphic mapping of $\mathcal{G}$ onto this group. The operators $\Phi(T)$ and the carrier space V are sometimes said to collectively form a "module". However, there is *no* guarantee that the operators are unitary for a given representation, that is, in general

$$(\Phi(T)\phi, \Phi(T)\psi) \neq (\phi, \psi).$$

(See Section 3 for further discussion of this point). Finally, if the basis is chosen to be an ortho-normal set, then Equation (4.1) implies that

$$\Gamma(T)_{mn} = (\psi_m, \Phi(T)\psi_n) \tag{4.4}$$

for any $T \in \mathcal{G}$. Conversely, any set of operators acting on a d-dimensional inner product space and satisfying Equation (4.3) will produce, by Equation (4.4), a d-dimensional matrix representation. (This provides the best way of introducing infinite-dimensional representations, the finite-dimensional inner product space merely being replaced by an infinite-dimensional Hilbert space, but these will not be discussed in this book.)

It is entirely a matter of taste and convenience whether one works with an explicit matrix representation or with the corresponding module consisting of the operators $\Phi(T)$ and the carrier space V on which they act. Theoretical physicists normally prefer to deal with the more concrete matrix representations, whereas pure mathematicians tend to prefer the module formulation.

It should be noted that for groups of coordinate transformations in $\mathbb{R}^3$, for which both the operators $\Phi(T)$ and $P(T)$ are defined, there are two major differences between these sets of operators. Firstly, the $\Phi(T)$ depend on the representation $\mathbf{\Gamma}$ under consideration, whereas the $P(T)$ are independent of the representation. Secondly, the operators $\Phi(T)$ act in a finite-dimensional space, whereas the $P(T)$ act in the infinite-dimensional Hilbert space L^2.

As the theory is developed in this chapter it will become apparent that every group has an infinite number of different representations, but these can be formed out of certain basic representations, the so-called "irreducible representations". For a finite group there is essentially only a finite number of these.

It will have become evident already that vector spaces and inner product spaces play an important part in representation theory. Readers who are not very familiar with them are advised to study Appendix B before proceeding further.

2 Equivalent representations

Theorem I Let $\mathbf{\Gamma}$ be a d-dimensional representation of a group $\mathcal{G}$, and let $\mathbf{S}$ be any $d \times d$ non-singular matrix. Define for each $T \in \mathcal{G}$ a $d \times d$ matrix

$\mathbf{\Gamma}'(T)$ by

$$\mathbf{\Gamma}'(T) = \mathbf{S}^{-1}\mathbf{\Gamma}(T)\mathbf{S}. \tag{4.5}$$

Then this set of matrices also forms a d-dimensional representation of $\mathcal{G}$. The representations $\mathbf{\Gamma}$ and $\mathbf{\Gamma}'$ are said to be "equivalent", and the transformation in Equation (4.5) is called a "similarity transformation".

Proof For any $T_1, T_2 \in \mathcal{G}$, by Equations (1.25) and (4.5),

$$\begin{aligned}\mathbf{\Gamma}'(T_1)\mathbf{\Gamma}'(T_2) &= \mathbf{S}^{-1}\mathbf{\Gamma}(T_1)\mathbf{S}\mathbf{S}^{-1}\mathbf{\Gamma}(T_2)\mathbf{S} = \mathbf{S}^{-1}\mathbf{\Gamma}(T_1)\mathbf{\Gamma}(T_2)\mathbf{S} \\ &= \mathbf{S}^{-1}\mathbf{\Gamma}(T_1T_2)\mathbf{S} = \mathbf{\Gamma}'(T_1T_2).\end{aligned}$$

In Section 6 there will be given a simple direct test for the equivalence of two representations which does not require actually finding the matrix $\mathbf{S}$ that induces the similarity transformation.

As all 1×1 matrices commute, if $d = 1$ then $\mathbf{\Gamma}'(T) = \mathbf{\Gamma}(T)$ for all $T \in \mathcal{G}$ and for every 1×1 non-singular matrix $\mathbf{S}$. Thus two one-dimensional representations of $\mathcal{G}$ are either identical or are not equivalent.

For $d \geq 2$ the situation is not so simple. In general a similarity transformation will produce an equivalent representation whose matrices $\mathbf{\Gamma}'(T)$ are different from those of $\mathbf{\Gamma}(T)$. However, these differences are in a sense superficial, for it will become clear that to a very large extent equivalent representations have essentially the same content. The following theorem on basis functions provides the first indication of this.

Theorem II Let $\mathbf{\Gamma}$ be a d-dimensional representation of a group of coordinate transformations in $\mathbb{R}^3$, let $\psi_1(\mathbf{r}), \psi_2(\mathbf{r}), \ldots, \psi_d(\mathbf{r})$ be a set of basis functions of $\mathbf{\Gamma}$ and let $\mathbf{S}$ be any $d \times d$ non-singular matrix. Then the set of d linearly independent functions $\psi'_1(\mathbf{r}), \psi'_2(\mathbf{r}), \ldots, \psi'_d(\mathbf{r})$ defined by

$$\psi'_n(\mathbf{r}) = \sum_{m=1}^{d} S_{mn}\psi_m(\mathbf{r}), \tag{4.6}$$

for $n = 1, 2, \ldots, d$ form a set of basis functions for the equivalent representation $\mathbf{\Gamma}'$, where, for all $T \in \mathcal{G}$,

$$\mathbf{\Gamma}'(T) = \mathbf{S}^{-1}\mathbf{\Gamma}(T)\mathbf{S}. \tag{4.7}$$

Proof For any $T \in \mathcal{G}$, from Equations (1.18), (1.26) and (4.6),

$$P(T)\psi'_n(\mathbf{r}) = \sum_{m=1}^{d} S_{mn}\{P(T)\psi_m(\mathbf{r})\} = \sum_{m,p=1}^{d} S_{mn}\Gamma(T)_{pm}\psi_p(\mathbf{r}).$$

However, inverting Equation (4.6) gives

$$\psi_p(\mathbf{r}) = \sum_{q=1}^{d} (\mathbf{S}^{-1})_{qp}\psi'_q(\mathbf{r}).$$

Thus, from Equation (4.7),

$$P(T)\psi'_n(\mathbf{r}) = \sum_{m,p,q=1}^{d} (\mathbf{S}^{-1})_{qp}\Gamma(T)_{pm}S_{mn}\psi'_q(\mathbf{r}) = \sum_{q=1}^{d} \Gamma'(T)_{qn}\psi'_q(\mathbf{r}).$$

The functions $\psi_1(\mathbf{r})$, $\psi_2(\mathbf{r})$, ... , $\psi_d(\mathbf{r})$ form a basis for a complex d-dimensional inner product space. With the definition in Equation (4.6), the functions $\psi'_1(\mathbf{r})$, $\psi'_2(\mathbf{r})$, ... , $\psi'_d(\mathbf{r})$ form an *alternative* basis for the *same* space. Thus *the effect of a similarity transformation is merely to rearrange the basis of this space without changing the space itself.*

This result has particular significance for the solutions of the time-independent Schrödinger equation. It was shown in Chapter 1, Section 4, that the eigenfunctions of a d-fold degenerate energy eigenvalue form a basis for a d-dimensional representation Γ of the group of the Schrödinger equation. However, *any* d linearly independent linear combinations of these eigenfunctions also form a set of eigenfunctions belonging to the *same* eigenvalue, and there is no reason to prefer the original set to this new set, or vice versa. As the new set forms a basis for a representation equivalent to Γ, *the representation of the group of the Schrödinger equation that corresponds to an energy eigenvalue is determined only up to equivalence.*

This section will be concluded by stating the analogous theorem which is valid for the carrier space of any representation of *any* group.

Theorem III Let Γ be a d-dimensional representation of a group $\mathcal{G}$, let $\psi_1, \psi_2, \ldots, \psi_d$ be a basis of its carrier space and define the operators $\Phi(T)$ for all $T \in \mathcal{G}$ by Equation (4.1) and its extension (4.2). Let $\mathbf{S}$ be any $d \times d$ non-singular matrix. Then the set of d linearly independent vectors $\psi'_1, \psi'_2, \ldots, \psi'_d$ defined by

$$\psi'_n = \sum_{m=1}^{d} S_{mn}\psi_m,$$

(for $n = 1, 2, \ldots, d$) forms a basis for the equivalent representation $\mathbf{\Gamma}'$, where, for all $T \in \mathcal{G}$,

$$\mathbf{\Gamma}'(T) = \mathbf{S}^{-1}\mathbf{\Gamma}(T)\mathbf{S},$$

in the sense that

$$\Phi(T)\psi'_n = \sum_{m=1}^{d} \Gamma'(T)_{mn}\psi'_m$$

for all $T \in \mathcal{G}$ and $n = 1, 2, \ldots, d$.

Proof This is essentially identical in content to that given above.

Again $\psi_1, \psi_2, \ldots, \psi_d$ and $\psi'_1, \psi'_2, \ldots, \psi'_d$ are merely two different bases for the *same* carrier space.

3 Unitary representations

Definition *Unitary representation of a group*
A "unitary" representation of a group $\mathcal{G}$ is a representation $\mathbf{\Gamma}$ in which the matrices $\mathbf{\Gamma}(T)$ are unitary for every $T \in \mathcal{G}$.

The following theorems show the profound difference between compact and non-compact Lie groups and the affinity between compact Lie groups and finite groups.

Theorem I If $\mathcal{G}$ is a *finite* group or a *compact* Lie group then *every* representation of $\mathcal{G}$ is *equivalent* to a *unitary* representation.

Proof See, for example, Appendix C of Cornwell (1984).

It will be recalled that all the point groups and space groups of solid state physics are finite. Likewise, the rotation groups in three dimensions and the internal symmetry groups of elementary particles are compact Lie groups. Thus, in all these situations, advantage may be taken of the considerable simplifications that result from using representations that are unitary.

Although the technical definition of "simple" and "semi-simple" Lie groups must be deferred until Chapter 11, Section 2, this is the appropriate place to mention some relevant properties of their representations.

Theorem II If $\mathcal{G}$ is a *non-compact* simple Lie group then $\mathcal{G}$ possesses *no* finite-dimensional unitary representations apart from the trivial representations in which $\mathbf{\Gamma}(T) = \mathbf{1}$ for all $T \in \mathcal{G}$.

Proof This will be given in Chapter 12, Section 2.

A non-compact Lie group that is not simple may possess both unitary representations and representations that are not equivalent to unitary representations, as the following example shows.

Example I *The multiplicative group of positive real numbers*
This group was considered previously in Examples I of Chapter 3, Sections 1, 2 and 3. A typical element is $\exp y_1$, $-\infty < y_1 < \infty$. It has a set of one-dimensional unitary representations defined by

$$\mathbf{\Gamma}(\exp y_1) = [\exp(i\alpha y_1)],$$

where α is any fixed real number. It has also a set of one-dimensional non-unitary representations given by

$$\mathbf{\Gamma}(\exp y_1) = [\exp(\beta y_1)],$$

where β is any fixed real number. These latter representations, being one-dimensional, cannot be transformed by any similarity transformation into unitary representations.

Theorem III If $\mathcal{G}$ is a group of coordinate transformations in $\mathbb{R}^3$ and if the representation $\mathbf{\Gamma}$ of $\mathcal{G}$ possesses a set of basis functions, then $\mathbf{\Gamma}$ is unitary if the basis functions form an ortho-normal set.

Proof Suppose that the basis functions $\psi_1(\mathbf{r}), \psi_2(\mathbf{r}), \ldots, \psi_d(\mathbf{r})$ of $\mathbf{\Gamma}$ form an ortho-normal set, i.e. $(\psi_m, \psi_n) = \delta_{mn}$ for $m, n = 1, 2, \ldots, d$. As the operators $P(T)$ are unitary, it follows from Equations (1.19), (1.20) and (1.26) that for each $T \in \mathcal{G}$

$$\begin{aligned} \delta_{mn} = (\psi_m, \psi_n) &= (P(T)\psi_m, P(T)\psi_n) \\ &= \sum_{p,q=1}^{d} \Gamma(T)^*_{pm} \Gamma(T)_{qn} (\psi_p, \psi_q) \\ &= \sum_{p,q=1}^{d} \Gamma(T)^*_{pm} \Gamma(T)_{pn}, \end{aligned}$$

so that $\mathbf{\Gamma}(T)^\dagger \mathbf{\Gamma}(T) = \mathbf{1}$ and hence $\mathbf{\Gamma}(T)$ is unitary.

From a set of basis functions $\psi_1(\mathbf{r}), \psi_2(\mathbf{r}), \ldots, \psi_d(\mathbf{r})$ of a non-unitary representation $\mathbf{\Gamma}$ an ortho-normal set $\psi'_1(\mathbf{r}), \psi'_2(\mathbf{r}), \ldots, \psi'_d(\mathbf{r})$ can always be constructed by the Schmidt orthogonalization process (see Appendix B, Section 2). As each $\psi'_j(\mathbf{r})$ is a linear combination of the $\psi_k(\mathbf{r})$, the set $\psi'_1(\mathbf{r})$, $\psi'_2(\mathbf{r}), \ldots,$ $\psi'_d(\mathbf{r})$ must be basis functions for a unitary representation $\mathbf{\Gamma}'$ that is equivalent to $\mathbf{\Gamma}$. Indeed, on defining the coefficients S_{mn} by $\psi'_n(\mathbf{r}) = \sum_{m=1}^{d} S_{mn}\psi_m(\mathbf{r})$, the matrix $\mathbf{S}$ having these coefficients as elements is precisely the matrix that induces the similarity transformation from $\mathbf{\Gamma}$ to $\mathbf{\Gamma}'$.

However, there exist groups of coordinate transformations in $\mathbb{R}^3$ that have at least some representations that do *not* possess basis functions, so this argument does *not* imply that every representation of every group of coordinate transformations is equivalent to a unitary representation.

For any abstract group $\mathcal{G}$ there exists a generalization of the last theorem. If an ortho-normal basis is used in the construction of the operators $\Phi(T)$ of Equations (4.1) and (4.3), it follows by an argument similar to that given in the above proof that, for each $T \in \mathcal{G}$, $\Phi(T)$ is a unitary operator if and only if $\mathbf{\Gamma}(T)$ is a unitary matrix.

The amount of attention that has just been devoted to non-unitary representations should not be allowed to obscure the main point, which is that in most cases of physical interest all the representations can be chosen to be unitary.

This section will be concluded with an important theorem that demonstrates the special role played in similarity transformations by matrices that

are unitary. (As noted in Appendix B, Section 2, such transformations transform ortho-normal bases into ortho-normal bases.)

Theorem IV If $\mathbf{\Gamma}$ and $\mathbf{\Gamma}'$ are two equivalent representations of a group $\mathcal{G}$ related by the similarity transformation

$$\mathbf{\Gamma}'(T) = \mathbf{S}^{-1}\mathbf{\Gamma}(T)\mathbf{S}$$

for all $T \in \mathcal{G}$, and if $\mathbf{\Gamma}$ is a unitary representation and $\mathbf{S}$ is a unitary matrix, then $\mathbf{\Gamma}'$ is also a unitary representation. Conversely, if $\mathbf{\Gamma}$ and $\mathbf{\Gamma}'$ are equivalent representations that are both unitary, then the matrix $\mathbf{S}$ in the similarity transformation relating them can always be chosen to be unitary.

Proof The first proposition is almost obvious, but the converse requires a rather lengthy proof, which may found, for example, in Appendix C of Cornwell (1984).

4 Reducible and irreducible representations

Suppose that the d-dimensional representation $\mathbf{\Gamma}$ of a group $\mathcal{G}$ can be partitioned so that it has the form

$$\mathbf{\Gamma}(T) = \begin{bmatrix} \mathbf{\Gamma}_{11}(T) & \mathbf{\Gamma}_{12}(T) \\ \mathbf{0} & \mathbf{\Gamma}_{22}(T) \end{bmatrix} \tag{4.8}$$

for every $T \in \mathcal{G}$, where $\mathbf{\Gamma}_{11}(T)$, $\mathbf{\Gamma}_{12}(T)$, $\mathbf{\Gamma}_{22}(T)$ and the zero matrix $\mathbf{0}$ have dimensions $s_1 \times s_1$, $s_1 \times s_2$, $s_2 \times s_2$ and $s_2 \times s_1$ respectively. (Here $s_1 + s_2 = d$, $s_1 \geq 1$, $s_2 \geq 1$ and s_1 and s_2 are the same for all $T \in \mathcal{G}$.) Then (cf. Equation (A.7)) for any $T_1, T_2 \in \mathcal{G}$

$$\mathbf{\Gamma}(T_1)\mathbf{\Gamma}(T_2) = \begin{bmatrix} \mathbf{\Gamma}_{11}(T_1)\mathbf{\Gamma}_{11}(T_2) & \mathbf{\Gamma}_{11}(T_1)\mathbf{\Gamma}_{12}(T_2) + \mathbf{\Gamma}_{12}(T_1)\mathbf{\Gamma}_{22}(T_2) \\ \mathbf{0} & \mathbf{\Gamma}_{22}(T_1)\mathbf{\Gamma}_{22}(T_2) \end{bmatrix},$$

so that, as the matrices $\mathbf{\Gamma}(T)$ form a representation of $\mathcal{G}$,

$$\mathbf{\Gamma}_{11}(T_1T_2) = \mathbf{\Gamma}_{11}(T_1)\mathbf{\Gamma}_{11}(T_2) \tag{4.9}$$

and

$$\mathbf{\Gamma}_{22}(T_1T_2) = \mathbf{\Gamma}_{22}(T_1)\mathbf{\Gamma}_{22}(T_2). \tag{4.10}$$

Equations (4.9) and (4.10) imply that the matrices $\mathbf{\Gamma}_{11}(T)$ and the matrices $\mathbf{\Gamma}_{22}(T)$ both form representations of $\mathcal{G}$. Thus the representation $\mathbf{\Gamma}$ of $\mathcal{G}$ is made up of two other representations of smaller dimensions, so it is natural to describe such a representation as being "reducible". In order that this description should apply equally to all equivalent representations, the formal definition can be stated as follows:

Definition *Reducible representation of a group* $\mathcal{G}$
A representation of a group $\mathcal{G}$ is said to be "reducible" if it is *equivalent* to a representation $\mathbf{\Gamma}$ of $\mathcal{G}$ that has the form of Equation (4.8) for all $T \in \mathcal{G}$.

It follows from Equations (4.1) and (4.8) that

$$\Phi(T)\psi_n = \sum_{m=1}^{s_1} \Gamma_{11}(T)_{mn}\psi_n,$$

for $n = 1, 2, \ldots, s_1$ and all $T \in \mathcal{G}$. Thus the s_1-dimensional subspace of the carrier space V having basis ψ_1, ψ_2, ... , ψ_{s_1} is invariant under all the operations of $\mathcal{G}$ in the sense that if ψ is any vector of this subspace then $P(T)\psi$ is also a member of this subspace for all $T \in \mathcal{G}$. (It should be noted that in general the s_2-dimensional subspace with basis $\psi_{s_1+1}, \psi_{s_1+2}, \ldots, \psi_d$ is *not* invariant.)

The following definition is the most important in the whole of the theory of representations.

Definition *Irreducible representation of a group* $\mathcal{G}$
A representation of a group $\mathcal{G}$ is said to be "irreducible" if it is not reducible.

This definition implies that an irreducible representation *cannot* be transformed by a similarity transformation to the form of Equation (4.8). Consequently the carrier space V of an irreducible representation has no invariant subspace of smaller dimension. Some simple tests for irreducibility will be developed in Sections 5 and 6.

Returning to the reducible representation $\mathbf{\Gamma}$ of Equation (4.8), the question arises as to whether $\mathbf{\Gamma}_{11}(T)$ and $\mathbf{\Gamma}_{22}(T)$ are also reducible or not. If $\mathbf{\Gamma}_{11}(T)$ is reducible, then by a similarity transformation it too can be put in the form of Equation (4.8) with submatrices of some dimensions. The same is true of $\mathbf{\Gamma}_{22}(T)$. Obviously this process can be continued until all the representations involved are irreducible. Thus every reducible representation $\mathbf{\Gamma}$ by an appropriate similarity transformation $\mathbf{S}$ can be put into the form

$$\mathbf{\Gamma}'(T) = \mathbf{S}^{-1}\mathbf{\Gamma}(T)\mathbf{S} = \begin{bmatrix} \mathbf{\Gamma}'_{11}(T) & \mathbf{\Gamma}'_{12}(T) & \mathbf{\Gamma}'_{13}(T) & \ldots & \mathbf{\Gamma}'_{1r}(T) \\ \mathbf{0} & \mathbf{\Gamma}'_{22}(T) & \mathbf{\Gamma}'_{23}(T) & \ldots & \mathbf{\Gamma}'_{2r}(T) \\ \mathbf{0} & \mathbf{0} & \mathbf{\Gamma}'_{33}(T) & \ldots & \mathbf{\Gamma}'_{3r}(T) \\ \vdots & \vdots & \vdots & & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \ldots & \mathbf{\Gamma}'_{rr}(T) \end{bmatrix},$$

where *all* the matrices $\mathbf{\Gamma}'_{jj}(T)$ form *irreducible* representations, for $j = 1, 2, \ldots, r$. (Here $\mathbf{\Gamma}'_{jk}(T)$ is an $s'_j \times s'_k$, matrix, $\sum_{j=1}^{r} s'_j = d$, $s'_j \geq 1$ for each $j = 1, 2, \ldots, r$, and $s'_1, s'_2, \ldots, s'_r$ are the same for all $T \in \mathcal{G}$.) *It is now apparent that the irreducible representations are the basic building blocks from which all reducible representations can be constructed.*

The final question is whether all the upper off-diagonal submatrices $\mathbf{\Gamma}'_{jk}(T)$ $(k > j)$ can be transformed into zero matrices by a further similarity transformation, leaving only the diagonal submatrices non-zero. If so, $\mathbf{\Gamma}$ is equivalent

to a representation of the form

$$\Gamma''(T) = \begin{bmatrix} \Gamma''_{11}(T) & \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \Gamma''_{22}(T) & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \Gamma''_{33}(T) & \dots & \mathbf{0} \\ \vdots & \vdots & \vdots & & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & \Gamma''_{rr}(T) \end{bmatrix}, \tag{4.11}$$

in which the Γ''_{jj} are all *irreducible* representations of $\mathcal{G}$.

Definition *Completely reducible representations of a group* $\mathcal{G}$
A representation Γ of a group $\mathcal{G}$ is said to be "completely reducible" if it is equivalent to a representation Γ'' that has the form in Equation (4.11) for all $T \in \mathcal{G}$.

A completely reducible representation is sometimes referred to as a "decomposable" representation.

Theorem I If $\mathcal{G}$ is a *finite* group or a *compact* Lie group then *every* reducible representation of $\mathcal{G}$ is *completely reducible.* The same is true of every reducible representation of a connected, non-compact, semi-simple Lie group and of any *unitary* reducible representation of any other group.

Proof See, for example, Chapter 4, Section 4, of Cornwell (1984).

Suppose that $\phi_1, \phi_2, \dots, \phi_d$ form a basis for the carrier space of the completely reducible representation Γ'' of Equation (4.11) and that the irreducible representation Γ''_{jj} has dimension d_j, $j = 1, 2, \dots, r$, so that $\sum_{j=1}^{r} d_j = d$. Then it follows from Equations (4.1) and (4.11) that $\phi_1, \phi_2, \dots, \phi_{d_1}$ form a basis for the carrier space of Γ''_{11}, that $\phi_{d_1+1}, \phi_{d_1+2}, \dots, \phi_{d_1+d_2}$ form a basis for the carrier space of Γ''_{22}, and so on. The carrier space of Γ'' is therefore a direct sum of carrier spaces belonging to each of the irreducible representations $\Gamma''_{11}, \Gamma''_{22}, \dots, \Gamma''_{rr}$ (see Appendix B, Section 1). Correspondingly, the completely reducible representation Γ'' is said to be the "direct sum" of the irreducible representations $\Gamma''_{11}, \Gamma''_{22}, \dots, \Gamma''_{rr}$, this statement being expressed concisely by

$$\Gamma'' = \Gamma''_{11} \oplus \Gamma''_{22} \oplus \dots \oplus \Gamma''_{rr}.$$

(The symbol $\oplus$ here indicates that the sum involved is *not* that of ordinary matrix addition.) Similarly, the equivalence of a representation Γ to a direct sum of irreducible representations $\Gamma''_{11}, \Gamma''_{22}, \dots, \Gamma''_{rr}$ can be written as

$$\Gamma \approx \Gamma''_{11} \oplus \Gamma''_{22} \oplus \dots \oplus \Gamma''_{rr}.$$

In the case in which Γ is equivalent to a unitary representation, all the irreducible representations in the direct sum are themselves equivalent to unitary representations.

5 Schur's Lemmas and the orthogonality theorem for matrix representations

The name "Schur's Lemma" is often attached to one or other (or sometimes both) of the following two theorems.

Theorem I Let $\mathbf{\Gamma}$ and $\mathbf{\Gamma}'$ be two *irreducible* representations of a group $\mathcal{G}$, of dimensions d and d' respectively, and suppose that there exists a $d \times d'$ matrix $\mathbf{A}$ such that

$$\mathbf{\Gamma}(T)\mathbf{A} = \mathbf{A}\mathbf{\Gamma}'(T)$$

for all $T \in \mathcal{G}$. Then *either* $\mathbf{A} = \mathbf{0}$, *or* $d = d'$ and $\det \mathbf{A} \neq 0$.

Proof See, for example, Appendix C, Section 3, of Cornwell (1984).

Theorem II If $\mathbf{\Gamma}$ is a d-dimensional *irreducible* representation of a group $\mathcal{G}$ and $\mathbf{B}$ is a $d \times d$ matrix such that $\mathbf{\Gamma}(T)\mathbf{B} = \mathbf{B}\mathbf{\Gamma}(T)$ for every $T \in \mathcal{G}$, then $\mathbf{B}$ must be a multiple of the unit matrix.

Proof Let $\mathbf{A} = \mathbf{B} - \beta\mathbf{1}$, where the complex number β is chosen so that $\det \mathbf{A} = 0$. Then $\mathbf{\Gamma}(T)\mathbf{A} = \mathbf{A}\mathbf{\Gamma}(T)$ for all $T \in \mathcal{G}$, so by the previous theorem the only alternative not excluded is $\mathbf{A} = \mathbf{0}$, that is, $\mathbf{B} = \beta\mathbf{1}$.

The following corollary shows how very straightforward are the irreducible representations of Abelian groups.

Theorem III Every irreducible representation of an *Abelian* group is *one*-dimensional.

Proof Let $\mathbf{\Gamma}$ be an irreducible representation of an Abelian group $\mathcal{G}$. As $\mathbf{\Gamma}(T)\mathbf{\Gamma}(T') = \mathbf{\Gamma}(T')\mathbf{\Gamma}(T)$ for all T and T' of $\mathcal{G}$, it follows from the preceding theorem that, for each $T' \in \mathcal{G}$, $\mathbf{\Gamma}(T') = \gamma(T')\mathbf{1}$, where $\gamma(T')$ is some complex number that depends on T'. Clearly, such a representation is irreducible if and only if it is one-dimensional.

The "orthogonality theorem for matrix representations" is a second corollary which will be used time and time again. As will be seen, it applies both to finite groups and compact Lie groups.

Theorem IV Suppose that $\mathbf{\Gamma}^p$ and $\mathbf{\Gamma}^q$ are two *unitary irreducible* representations of a finite group $\mathcal{G}$ which are not equivalent if $p \neq q$ (but which are identical if $p = q$). Then

$$(1/g)\sum_{T\in\mathcal{G}} \Gamma^p(T)^\star_{jk}\Gamma^q(T)_{st} = (1/d_p)\delta_{pq}\delta_{js}\delta_{kt},$$

where g is the order of $\mathcal{G}$ and d_p is the dimension of $\mathbf{\Gamma}^p$. Similarly, if $\mathcal{G}$ is a compact Lie group, the summation can be replaced by an invariant integration,

giving

$$\int_{\mathcal{G}} \Gamma^p(T)^\star_{jk} \Gamma^q(T)_{st}\, dT = (1/d_p)\delta_{pq}\delta_{js}\delta_{kt}.$$

Proof See, for example, Appendix C, Section 3, of Cornwell (1984).

It is in the application of this theorem that the main practical advantage of working with unitary representations lies. For example, one immediate consequence is the following partial converse to Theorem III of Section 3.

Theorem V If $\phi_1^p(\mathbf{r}), \phi_2^p(\mathbf{r}), \ldots$, and $\psi_1^q(\mathbf{r}), \psi_2^q(\mathbf{r}), \ldots$, are respectively basis functions for the *unitary irreducible* representations $\mathbf{\Gamma}^p$ and $\mathbf{\Gamma}^q$ of a group of coordinate transformations $\mathcal{G}$ that is either a finite group or a compact Lie group, and $\mathbf{\Gamma}^p$ and $\mathbf{\Gamma}^q$ are not equivalent if $p \neq q$ (but are identical if $p = q$), then

$$(\phi_m^p, \psi_n^q) = 0$$

unless $p = q$ and $m = n$. If $p = q$ and $m = n$, then (ϕ_m^p, ψ_m^p) is a constant independent of m.

Proof From Equations (1.20) and (1.26), for any $T \in \mathcal{G}$,

$$\begin{aligned}(\phi_m^p, \psi_n^q) &= (P(T)\phi_m^p, P(T)\psi_n^q) \\ &= \sum_{j=1}^{d_p}\sum_{k=1}^{d_q} \Gamma^p(T)^\star_{jm}\Gamma^q(T)_{kn}(\phi_j^p, \psi_k^q),\end{aligned}$$

d_p and d_q being the dimensions of $\mathbf{\Gamma}^p$ and $\mathbf{\Gamma}^q$ respectively. Summing or integrating over all the transformations $T \in \mathcal{G}$, the orthogonality theorem for matrix representations gives

$$(\phi_m^p, \psi_n^q) = (1/d_p)\delta_{pq}\delta_{mn}\sum_{j=1}^{d_p}(\phi_j^p, \psi_j^p).$$

Thus when $p \neq q$, or when $p = q$ but $m \neq n$, it follows immediately that $(\phi_m^p, \psi_n^q) = 0$. When $p = q$ and $m = n$ the right-hand side of this last equation is independent of m, so (ϕ_m^p, ψ_m^p) must be independent of m.

One immediate implication of this theorem is that

$$(\phi_m^p, \psi_n^p) = \delta_{mn}(\phi_1^p, \psi_1^p)$$

for all $m, n = 1, 2, \ldots, d_p$. Thus, if $\psi_1^p(\mathbf{r})$ is normalized, then so too are $\psi_2^p(\mathbf{r}), \psi_3^p(\mathbf{r}), \ldots$. Henceforth it will usually be assumed that every set of basis functions of an irreducible representation is a mutually ortho-normal set, that is,

$$(\phi_m^p, \psi_n^p) = \delta_{mn}$$

for all $m, n = 1, 2, \ldots, d_p$.

6 Characters

Although equivalent representations have essentially the same content, there is a large degree of arbitrariness in the explicit forms of their matrices. However, the characters provide a set of quantities which are the same for all equivalent representations. Indeed, for finite groups and compact Lie groups the characters *uniquely* determine the representations up to equivalence.

The characters have a number of other very useful properties which, for the most part, are valid for finite groups or compact Lie groups but not for non-compact Lie groups.

Definition *Characters of a representation*
Suppose that $\mathbf{\Gamma}$ is a d-dimensional representation of a group $\mathcal{G}$. Then

$$\chi(T) = \text{tr } \mathbf{\Gamma}(T) \quad (= \sum_{j=1}^{d} \Gamma(T)_{jj})$$

is defined to be the "character" of the group element T in this representation. The set of characters corresponding to a representation is called the "character system" of the representation.

As $\mathbf{\Gamma}(E) = \mathbf{1}_d$ for the identity E of $\mathcal{G}$, then $\chi(E) = d$.

Theorem I A necessary condition for two representations of a group to be equivalent is that they must have identical character systems.

Proof Let $\mathbf{\Gamma}$ and $\mathbf{\Gamma}'$ be two equivalent representations of a group $\mathcal{G}$, both of dimension d, so that there exists a $d \times d$ non-singular matrix $\mathbf{S}$ such that $\mathbf{\Gamma}'(T) = \mathbf{S}^{-1}\mathbf{\Gamma}(T)\mathbf{S}$ for all $T \in \mathcal{G}$. Then, as noted in Appendix A, tr $\mathbf{\Gamma}'(T) =$ tr $\mathbf{\Gamma}(T)$. Thus, if $\chi(T)$ and $\chi'(T)$ are the characters of T in $\mathbf{\Gamma}$ and $\mathbf{\Gamma}'$ respectively, then $\chi'(T) = \chi(T)$ for all $T \in \mathcal{G}$.

The characters therefore provide a set of quantities that are unchanged by similarity transformations. The converse proposition will be considered shortly. The invariance property of the trace also provides another simple result:

Theorem II In a given representation of a group $\mathcal{G}$, all the elements in the same class have the same character.

Proof Suppose that the elements T' and T of $\mathcal{G}$ are in the same class. Then (see Chapter 2, Section 2) there exists a group element X such that $T' = XTX^{-1}$, so that $\mathbf{\Gamma}(T') = \mathbf{\Gamma}(X)\mathbf{\Gamma}(T)\mathbf{\Gamma}(X)^{-1}$. Consequently tr $\mathbf{\Gamma}'(T) =$ tr $\mathbf{\Gamma}(T)$, and hence $\chi'(T) = \chi(T)$.

There are two orthogonality theorems for characters. The first is as follows:

Theorem III Let $\chi^p(T)$ and $\chi^q(T)$ be the characters of two irreducible representations of a finite group $\mathcal{G}$ of order g, these representations being assumed to be inequivalent if $p \neq q$. Then

$$(1/g) \sum_{T \in \mathcal{G}} \chi^p(T)^* \chi^q(T) = \delta_{pq}.$$

Similarly, if $\mathcal{G}$ is a compact Lie group, the summation can be replaced by an invariant integration, giving

$$\int_{\mathcal{G}} \chi^p(T)^* \chi^q(T)\, dT = \delta_{pq}.$$

Proof Theorem I of Section 3 shows that for the groups under consideration similarity transformations may be applied to the two irreducible representations to produce unitary representations. The result then follows immediately from the orthogonality theorem for matrix representations (Theorem IV of Section 5) on putting $j = k$ and $s = t$ and summing over j and s.

The converse theorem referred to previously can now be proved fairly easily.

Theorem IV If $\mathcal{G}$ is a *finite* group or a *compact* Lie group then a sufficient condition for two representations to be equivalent is provided by the equality of their character systems.

Proof See, for example, Appendix C, Section 4, of Cornwell (1984).

It should be noted that this sufficient condition does *not* extend to *non-compact* Lie groups.

The characters provide a complete specification (up to equivalence) of the irreducible representations that appear in a reducible representation. This knowledge can prove very useful, as will be seen later. The details are as given by the following theorem.

Theorem V The number of times n_p that an irreducible representation $\mathbf{\Gamma}^p$ (or a representation equivalent to $\mathbf{\Gamma}^p$) appears in a reducible representation $\mathbf{\Gamma}$ is given for a finite group $\mathcal{G}$ by

$$n_p = (1/g) \sum_{T \in \mathcal{G}} \chi(T) \chi^p(T)^*,$$

where $\chi^p(T)$ and $\chi(T)$ are the characters of $\mathbf{\Gamma}^p$ and $\mathbf{\Gamma}$ respectively and g is the order of $\mathcal{G}$. For a compact Lie group this generalizes to

$$n_p = \int_{\mathcal{G}} \chi(T) \chi^p(T)^*\, dT.$$

Proof See, for example, Chapter 4, Section 6, of Cornwell (1984).

The following theorem gives a convenient criterion for irreducibility expressed solely in terms of characters, and so provides a very simple test for irreducibility, particularly for finite groups.

Theorem VI A necessary and sufficient condition for a representation $\mathbf{\Gamma}$ of a finite group $\mathcal{G}$ to be *irreducible* is that

$$(1/g) \sum_{T \in \mathcal{G}} |\chi(T)|^2 = 1,$$

where $\chi(T)$ is the character of the group element T in $\mathbf{\Gamma}$ and g is the order of $\mathcal{G}$. The corresponding condition for a compact Lie group is

$$\int_{\mathcal{G}} |\chi(T)|^2 \, dT = 1.$$

Proof See, for example, Chapter 4, Section 6, of Cornwell (1984).

Characters may also be used to prove a theorem on the number of inequivalent irreducible representations of a finite group $\mathcal{G}$, as well as a useful result on their dimensions.

Theorem VII For a *finite* group $\mathcal{G}$, the sum of the squares of the dimensions of the inequivalent irreducible representations is equal to the order of $\mathcal{G}$.

Proof See, for example, Appendix C, Section 4, of Cornwell (1984).

Theorem VIII For a *finite* group $\mathcal{G}$, the number of inequivalent irreducible representations is equal to the number of classes of $\mathcal{G}$.

Proof See, for example, Appendix C, Section 4, of Cornwell (1984).

These two theorems taken together are often sufficient to uniquely specify the dimensions of the inequivalent irreducible representations.

Example I *Dimensions of the inequivalent irreducible representations of the crystallographic point group* D_4
As noted in Chapter 2, Section 2, D_4 is of order 8 and has five classes. Thus it has five inequivalent irreducible representations. Let d_j, $j = 1, 2, \ldots, 5$, be their dimensions, so that $\sum_{j=1}^{5} {d_j}^2 = 8$, which has the solution $d_1 = d_2 = d_3 = d_4 = 1$ and $d_5 = 2$. This solution is unique up to a relabelling of representations.

The second orthogonality theorem for characters is as follows.

Theorem IX If $\chi^p(\mathcal{C}_j)$ is the character of the class $\mathcal{C}_j$ of a finite group $\mathcal{G}$ for the irreducible representation $\mathbf{\Gamma}^p$ of $\mathcal{G}$, then

$$\sum_p \chi^p(\mathcal{C}_j)^\star \chi^p(\mathcal{C}_k) N_k = g\delta_{jk},$$

where the sum is over all the inequivalent irreducible representations of $\mathcal{G}$, g is the order of $\mathcal{G}$ and N_j is the number of elements in the class $\mathcal{C}_j$.

Proof See, for example, Appendix C, Section 4, of Cornwell (1984).

The character systems of the irreducible representations of a finite group are conveniently displayed in the form of a "character table". The classes of the group are usually listed along the top of the table and the inequivalent irreducible representations are listed down the left-hand side. As a consequence of the Theorem VIII above, this table is always square.

For groups of low order it is quite easy to completely determine the character table directly from the theorems that have just been stated, without first obtaining explicit forms for the matrices, as the following example will show.

Example II *Character table for the crystallographic point group* D_4
The classes of D_4 (see Chapter 2, Section 2) are $\mathcal{C}_1 = \{E\}$, $\mathcal{C}_2 = \{C_{2x}, C_{2z}\}$, $\mathcal{C}_3 = \{C_{2y}\}$, $\mathcal{C}_4 = \{C_{4y}, C_{4y}^{-1}\}$, $\mathcal{C}_5 = \{C_{2c}, C_{2d}\}$.

Consider first the four one-dimensional representations $\mathbf{\Gamma}^1$, $\mathbf{\Gamma}^2$, $\mathbf{\Gamma}^3$ and $\mathbf{\Gamma}^4$. As $C_{2x}^2 = C_{2c}^2 = E$ then $\chi^p(C_{2x})^2 = \chi^p(C_{2c})^2 = 1$, $p = 1, 2, 3, 4$. Moreover, from Table 1.2, $C_{4y} = C_{2c}C_{2x}$, so that $\chi^p(\mathcal{C}_4) = \chi^p(\mathcal{C}_2)\chi^p(\mathcal{C}_5)$. Finally, $C_{2y} = C_{4y}^2$, so $\chi^p(C_{2y}) = 1$ for $p = 1, 2, 3, 4$. Thus the four one-dimensional irreducible representations of D_4 may be chosen to be such that: $\chi^1(\mathcal{C}_2) = 1$, $\chi^1(\mathcal{C}_5) = 1$; $\chi^2(\mathcal{C}_2) = 1$, $\chi^2(\mathcal{C}_5) = -1$; $\chi^3(\mathcal{C}_2) = -1$, $\chi^3(\mathcal{C}_5) = -1$; $\chi^4(\mathcal{C}_2) = -1$, $\chi^4(\mathcal{C}_5) = 1$.

From the first orthogonality theorem for characters (Theorem III) the two-dimensional representation $\mathbf{\Gamma}^5$ must satisfy the conditions:

$$\left.\begin{aligned}
\chi^5(\mathcal{C}_1) + 2\chi^5(\mathcal{C}_2) + \chi^5(\mathcal{C}_3) + 2\chi^5(\mathcal{C}_4) + 2\chi^5(\mathcal{C}_5) &= 0,\\
\chi^5(\mathcal{C}_1) + 2\chi^5(\mathcal{C}_2) + \chi^5(\mathcal{C}_3) - 2\chi^5(\mathcal{C}_4) - 2\chi^5(\mathcal{C}_5) &= 0,\\
\chi^5(\mathcal{C}_1) - 2\chi^5(\mathcal{C}_2) + \chi^5(\mathcal{C}_3) + 2\chi^5(\mathcal{C}_4) - 2\chi^5(\mathcal{C}_5) &= 0,\\
\chi^5(\mathcal{C}_1) - 2\chi^5(\mathcal{C}_2) + \chi^5(\mathcal{C}_3) - 2\chi^5(\mathcal{C}_4) + 2\chi^5(\mathcal{C}_5) &= 0.
\end{aligned}\right\}$$

Adding these equations gives $\chi^5(\mathcal{C}_1) + \chi^5(\mathcal{C}_3) = 0$ and, as $\chi^5(\mathcal{C}_1) = \chi^5(E) = 2$, this implies $\chi^5(\mathcal{C}_3) = -2$. Moreover, Theorem VI above gives $\sum_{T\in\mathcal{G}} |\chi^5(T)|^2 = 8$, while $|\chi^5(E)|^2 + |\chi^5(C_{2y})|^2 = 8$, so that $\chi^5(\mathcal{C}_2) = \chi^5(\mathcal{C}_4) = \chi^5(\mathcal{C}_5) = 0$.

The complete character table for D_4 is given in Table 4.1. It is interesting to relate these irreducible representations to the representations of D_4 discussed in Example I of Section 1. $\mathbf{\Gamma}^1$ is clearly the "identity" representation (iv), $\mathbf{\Gamma}^2$ is the one-dimensional representation (iii), $\mathbf{\Gamma}^5$ is the two-dimensional representation (ii), and the three-dimensional representation (i) is reducible, being given by the direct sum $\mathbf{\Gamma}^3 \oplus \mathbf{\Gamma}^5$.

	E	C_{2x}, C_{2z}	C_{2y}	C_{4y}, C_{4y}^{-1}	C_{2c}, C_{2d}
$\mathbf{\Gamma}^1$	1	1	1	1	1
$\mathbf{\Gamma}^2$	1	1	1	-1	-1
$\mathbf{\Gamma}^3$	1	-1	1	1	-1
$\mathbf{\Gamma}^4$	1	-1	1	-1	1
$\mathbf{\Gamma}^5$	2	0	-2	0	0

Table 4.1: Character table for the crystallographic point group D_4.

Although a number of results of physical significance follow immediately from a knowledge of the characters, it is often necessary to obtain explicit expressions for the matrices of the representations. A method for constructing such explicit expressions from the characters is described in Chapter 5, Section 1. Of course, for one-dimensional representations the characters themselves are the matrix elements.

Hitherto all results on finite groups have had an immediate generalization for compact Lie groups. For Theorems VII and VIII above this generalization is more far-reaching and is embodied in the following theorem due to Peter and Weyl (1927).

Theorem X For a *compact* Lie group $\mathcal{G}$, the number of inequivalent irreducible representations is infinite but *countable.*

This theorem implies that the irreducible representations of a compact Lie group can be specified by a parameter that only takes *integral* values (or, if more convenient, by a set of parameters taking integral values). This result has been anticipated in some of the notations already employed (but not in any of the proofs).

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Chapter 5

Representations of Groups - Developments

Having laid the foundations of the theory of group representations in the previous chapter, attention will now be concentrated on certain developments that are particularly significant in the applications to quantum mechanics.

1 Projection operators

For any *finite* group $\mathcal{G}$ of coordinate transformations in $\mathbb{R}^3$, in particular for any crystallographic point group or space group, the basis functions of unitary irreducible representations are easily determined by a purely automatic process involving certain "projection operators". Before defining these it is necessary to state a theorem which has many applications.

Theorem I Any function $\phi(\mathbf{r})$ of L^2 can be written as a linear combination of basis functions of the unitary irreducible representations of a group $\mathcal{G}$ of coordinate transformations in $\mathbb{R}^3$. That is

$$\phi(\mathbf{r}) = \sum_p \sum_{j=1}^{d_p} a_j^p \phi_j^p(\mathbf{r}), \tag{5.1}$$

where $\phi_j^p(\mathbf{r})$ is a normalized basis function transforming as the jth row of the d_p-dimensional unitary irreducible representation $\mathbf{\Gamma}^p$ of $\mathcal{G}$, a_j^p are a set of complex numbers and the sum over p is over all the inequivalent unitary irreducible representations of $\mathcal{G}$.

Here L^2 is the space of square-integrable functions, as defined in Appendix B, Section 3. The basis functions $\phi_j^p(\mathbf{r})$ and coefficients a_j^p depend on $\phi(\mathbf{r})$ and some of the coefficients a_j^p may be zero. For example, for the crystallographic point group D_4 it will be demonstrated in Example I below

that with the choice $\phi(\mathbf{r}) = (x+z)\exp(-r)$ (where $r = \{x^2+y^2+z^2\}^{1/2}$), $\phi(\mathbf{r}) = A^{-1}\{\phi_1^5(\mathbf{r})+\phi_2^5(\mathbf{r})\}$ with $\phi_1^5(\mathbf{r}) = Ax\exp(-r)$ and $\phi_2^5(\mathbf{r}) = Az\exp(-r)$, whereas with $\phi(\mathbf{r}) = y(x+z)\exp(-r)$, $\phi(\mathbf{r}) = B^{-1}\{\phi_1^5(\mathbf{r}) - \phi_2^5(\mathbf{r})\}$ with $\phi_1^5(\mathbf{r}) = Byz\exp(-r)$ and $\phi_2^5(\mathbf{r}) = -Bxy\exp(-r)$.

There is no suggestion in the theorem that the functions $\phi_j^p(\mathbf{r})$ on the right-hand side of Equation (5.1) form a *fixed* basis for the space L^2. Indeed this would be impossible for a finite group as L^2 is infinite-dimensional, whereas there is only a finite number of functions on the right-hand side of Equation (5.1) when $\mathcal{G}$ is a finite group. On the other hand, the theorem can be applied to every member of a complete basis for the space L^2 in turn, thereby producing a basis for L^2, all of whose members are basis functions of unitary irreducible representations of $\mathcal{G}$. A situation where this proves very useful is examined in Chapter 6, Section 1.

Proof See, for example, Appendix C, Section 5, of Cornwell (1984).

Definition *Projection operators*
Let $\mathbf{\Gamma}^p$ be a unitary irreducible representation of dimension d_p of a finite group of coordinate transformations $\mathcal{G}$ of order g. Then the projection operators are defined by

$$\mathcal{P}_{mn}^p = (d_p/g)\sum_{T\in\mathcal{G}} \Gamma^p(T)_{mn}^* P(T), \tag{5.2}$$

for $m, n = 1, 2, \ldots, d_p$. If the group of coordinate transformations is a compact Lie group, the definition may be generalized to

$$\mathcal{P}_{mn}^p = d_p \int_{\mathcal{G}} \Gamma^p(T)_{mn}^* P(T)\, dT. \tag{5.3}$$

Theorem II The projection operators $\mathcal{P}_{mn}^p$ have the following properties:

(a) For any two functions $\phi(\mathbf{r})$ and $\psi(\mathbf{r})$ of L^2

$$(\mathcal{P}_{mn}^p\phi, \psi) = (\phi, \mathcal{P}_{nm}^p\psi). \tag{5.4}$$

In particular

$$(\mathcal{P}_{nn}^p\phi, \psi) = (\phi, \mathcal{P}_{nn}^p\psi), \tag{5.5}$$

so that $\mathcal{P}_{nn}^p$ is a self-adjoint operator.

(b) If the projection operators $\mathcal{P}_{mn}^p$ and $\mathcal{P}_{jk}^q$ belong to two unitary irreducible representations $\mathbf{\Gamma}^p$ and $\mathbf{\Gamma}^q$ of $\mathcal{G}$ that are not equivalent if $p \neq q$ (but are identical if $p = q$), then

$$\mathcal{P}_{mn}^p\mathcal{P}_{jk}^q = \delta_{pq}\delta_{nj}\mathcal{P}_{mk}^q. \tag{5.6}$$

In particular

$$(\mathcal{P}_{nn}^p)^2 = \mathcal{P}_{nn}^p. \tag{5.7}$$

(c) If $\psi_1^q(\mathbf{r}), \psi_2^q(\mathbf{r}), \ldots$, are basis functions transforming as the unitary irreducible representation $\mathbf{\Gamma}^q$ of $\mathcal{G}$, then

$$\mathcal{P}_{mn}^p \psi_j^q(\mathbf{r}) = \delta_{pq}\delta_{nj}\psi_m^p(\mathbf{r}). \tag{5.8}$$

(d) For any function $\phi(\mathbf{r})$ of L^2

$$\mathcal{P}_{nn}^p \phi(\mathbf{r}) = a_n^p \psi_n^p(\mathbf{r}), \tag{5.9}$$

where a_n^p and $\psi_n^p(\mathbf{r})$ are the coefficients and basis functions of the expansion of $\phi(\mathbf{r})$ (Equation (5.1)) that relate to the nth row of $\mathbf{\Gamma}^p$.

Proof See, for example, Appendix C, Section 5, of Cornwell (1984).

The properties in Equations (5.5) and (5.7) are characteristic of any projection operators. The nature of the projection associated with the operator $\mathcal{P}_{mn}^p$ is apparent from Equation (5.9), which shows that $\mathcal{P}_{nn}^p$ projects into the subspace of L^2 consisting of functions transforming as the nth row of $\mathbf{\Gamma}^p$. As operators with the property in Equation (5.7) are known as "idempotent" operators, the projection operator technique is sometimes called the "idempotent method".

For a finite group this theorem provides a simple automatic method for the construction of basis functions. (For a compact Lie group it is preferable to use other methods, as for example in Chapter 10, Section 4.) A set of ortho-normal basis functions transforming as the rows of $\mathbf{\Gamma}^p$ can be found by first selecting a function $\phi(\mathbf{r})$ such that $\mathcal{P}_{nn}^p \phi(\mathbf{r})$ is not identically zero for some arbitrarily chosen $n = 1, 2, \ldots, d_p$. With $c_n^p = (\mathcal{P}_{nn}^p \phi, \mathcal{P}_{nn}^p \phi)^{1/2}$, the function $\psi_n^p(\mathbf{r})$ defined by

$$\psi_n^p(\mathbf{r}) = (1/c_n^p)\mathcal{P}_{nn}^p \phi(\mathbf{r})$$

is normalized and transforms as the nth row of $\mathbf{\Gamma}^p$. Should its ortho-normal partners $\psi_m^p(\mathbf{r})$ $(m = 1, 2, \ldots, d_p; m \neq n)$ be required, they can be found by operating on $\psi_n^p(\mathbf{r})$ with $\mathcal{P}_{mn}^p$. It will be seen later (Chapter 6, Section 1) that in physical problems it is usually only necessary to work with basis functions belonging to one arbitrarily chosen row of each irreducible representation.

Example I *Construction of basis functions of irreducible representations of the crystallographic point group D_4*

First let $\phi(\mathbf{r}) = (x + z)\exp(-r)$, where $r = \{x^2 + y^2 + z^2\}^{1/2}$. Then, from Equations (1.8) and (1.17), for any pure rotation T,

$$P(T)\phi(\mathbf{r}) = \phi(\mathbf{R}(T)^{-1}\mathbf{r}) = \phi(\widetilde{\mathbf{R}}(T)\mathbf{r}),$$

the orthogonal matrices $\mathbf{R}(T)$ for D_4 being given in Example III of Chapter 1, Section 2. For example, for $T = C_{4y}$,

$$\widetilde{\mathbf{R}}(C_{4y})\mathbf{r} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} z \\ y \\ -x \end{bmatrix},$$

and as $\phi(\widetilde{\mathbf{R}}(C_{4y})\mathbf{r})$ is defined to be the function in which the x, y and z in $\phi(\mathbf{r})$ are replaced by the 11, 21 and 31 components of $\widetilde{\mathbf{R}}(C_{4y})\mathbf{r}$ respectively, and here $\phi(\mathbf{r}) = (x+z)\exp(-r)$, then

$$P(C_{4y})\phi(\mathbf{r}) = (z-x)\exp(-r).$$

The following is a complete list of functions $P(T)\phi(\mathbf{r})$ obtained in this way:

$$\left.\begin{array}{lllll} P(E)\phi(\mathbf{r}) & = & P(C_{2c})\phi(\mathbf{r}) & = & (x+z)\exp(-r), \\ P(C_{2x})\phi(\mathbf{r}) & = & P(C_{4y}^{-1})\phi(\mathbf{r}) & = & (x-z)\exp(-r), \\ P(C_{2y})\phi(\mathbf{r}) & = & P(C_{2d})\phi(\mathbf{r}) & = & (-x-z)\exp(-r), \\ P(C_{2z})\phi(\mathbf{r}) & = & P(C_{4y})\phi(\mathbf{r}) & = & (-x+z)\exp(-r). \end{array}\right\} \tag{5.10}$$

Being one-dimensional, the matrices of the irreducible representations $\mathbf{\Gamma}^1$, $\mathbf{\Gamma}^2$, $\mathbf{\Gamma}^3$ and $\mathbf{\Gamma}^4$ are given directly in terms of the characters of Table 4.1 by $\mathbf{\Gamma}^j(T) = [\chi^j(T)]$ for all T of D_4 and $j = 1,2,3,4$. As noted in Example II of Chapter 4, Section 6, the matrices of the two-dimensional irreducible representation $\mathbf{\Gamma}^5$ may be taken to be:

$$\mathbf{\Gamma}^5(E) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \mathbf{\Gamma}^5(C_{2x}) = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \mathbf{\Gamma}^5(C_{2y}) = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix},$$

$$\mathbf{\Gamma}^5(C_{2z}) = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \mathbf{\Gamma}^5(C_{4y}) = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \quad \mathbf{\Gamma}^5(C_{4y}^{-1}) = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix},$$

$$\mathbf{\Gamma}^5(C_{2c}) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \mathbf{\Gamma}^5(C_{2d}) = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}.$$

Then, by Equation (5.2), $\mathcal{P}_{11}^p\phi(\mathbf{r}) = 0$ for $p = 1,2,3,4$, whereas $\mathcal{P}_{11}^5\phi(\mathbf{r}) = x\exp(-r)$. Thus the function $Ax\exp(-r)$, where

$$A = (1/c_1^5) = (x\exp(-r), x\exp(-r))^{-1/2},$$

is a normalized basis function transforming as the first row of $\mathbf{\Gamma}^5$, its partner transforming as the second row of $\mathbf{\Gamma}^5$ is $\mathcal{P}_{21}^5\{Ax\exp(-r)\}$, which is equal to $Az\exp(-r)$.

It will be seen that, as $P(T)\exp(-r) = \exp(-r)$ for all $T \in \mathcal{G}$, the factor $\exp(-r)$ plays no role in the construction apart from ensuring that the basis functions can be normalized. Consequently, if $\exp(-r)$ is replaced by *any* function $F(r)$ such that $(xF(r), xF(r))$ is finite, then $A'xF(r)$ and $A'zF(r)$ (where $A' = (xF(r), xF(r))^{-1/2}$) are ortho-normal basis functions of $\mathbf{\Gamma}^5$ transforming as the first and second rows respectively. Clearly no harm comes from temporarily being less precise than usual and saying that "x and z transform as the first and second rows of $\mathbf{\Gamma}^5$". Such statements about basis functions of irreducible representations of groups of pure rotations appear quite commonly in the literature.

A similar analysis applied to $\phi(\mathbf{r}) = (xy+yz)\exp(-r)$ shows that $\mathcal{P}_{11}^p\phi(\mathbf{r}) = 0$ for $p = 1,2,3,4$, but $\mathcal{P}_{11}^5\phi(\mathbf{r}) = yz\exp(-r)$. Thus $Byz\exp(-r)$ (where $B = (1/c_1^5) = (yz\exp(-r), yz\exp(-r))^{-1/2}$) is a normalized basis function

transforming as the first row of $\mathbf{\Gamma}^5$. Its partner transforming as the second row of $\mathbf{\Gamma}^5$ is $\mathcal{P}^5_{21}\{Byz\exp(-r)\}$, which is equal to $-Bxy\exp(-r)$. Again, loosely one could say that "yz and $-xy$ transform as the first and second rows of $\mathbf{\Gamma}^5$".

The procedure for constructing basis functions that has just been described requires an explicit knowledge of the matrix elements of the representations, and not merely a knowledge of the character system alone, which is usually the only information which is given in the published literature. Of course, for one-dimensional representations the characters give the matrix elements immediately, but for the other representations some further analysis is needed. A method involving "character projection operators", which can be used in such cases, will now be described.

Definition *Character projection operator*
Let $\mathbf{\Gamma}^p$ be an irreducible representation of dimension d_p of a finite group of coordinate transformations $\mathcal{G}$ of order g, $\chi^p(T)$ being the character of $T \in \mathcal{G}$ in $\mathbf{\Gamma}^p$. Then the character projection operator for $\mathcal{P}^p$ is defined by

$$\mathcal{P}^p = (d_p/g)\sum_{T\in\mathcal{G}} \chi^p(T)^* P(T). \tag{5.11}$$

Obviously $\mathcal{P}^p$ can be constructed from the character table alone and

$$\mathcal{P}^p = \sum_{n=1}^{d_p} \mathcal{P}^p_{nn},$$

so that $\mathcal{P}^p$ has the property of projecting out of a function $\phi(\mathbf{r})$ the sum of *all* the parts transforming according to the rows of $\mathbf{\Gamma}^p$. This implies that if $\mathcal{P}^p\phi(\mathbf{r})$ is not identically zero, it is a linear combination of basis functions of $\mathbf{\Gamma}^p$ (which are as yet undetermined). However, as noted in Chapter 4, Section 2, linear combinations of basis functions are themselves basis functions in an equivalent representation, so $\mathcal{P}^p\phi(\mathbf{r})$ may be taken to transform as the first row of some form of the pth irreducible representation. This particular form will henceforth be denoted by $\mathbf{\Gamma}^p$. (Up to this stage $\mathbf{\Gamma}^p$ was only specified up to a similarity transformation.) The procedure to be described then generates explicit matrix elements for this form of $\mathbf{\Gamma}^p$, which is, of course, as good as any other equivalent form.

Having chosen a normalizable $\phi(\mathbf{r})$ such that $\mathcal{P}^p\phi(\mathbf{r})$ is not identically zero, construct $P(T)\{\mathcal{P}^p\phi(\mathbf{r})\}$ for each $T \in \mathcal{G}$. (Each of these must be linear combinations of the d_p basis functions of $\mathbf{\Gamma}^p$.) From these functions abstract d_p linearly independent functions, taking one of these to be $\mathcal{P}^p\phi(\mathbf{r})$ itself. Apply the Schmidt orthogonalization process (see Appendix B, Section 2) to these functions to produce d_p orthonormal functions $\psi^p_n(\mathbf{r})$, $n = 1, 2, \ldots, d_p$, $\psi^p_1(\mathbf{r})$ being a multiple of $\mathcal{P}^p\phi(\mathbf{r})$. These functions can be taken as the basis

functions of a unitary representation of $\mathbf{\Gamma}^p$. The matrix elements can then be found from Equation (1.26), that is, from

$$P(T)\psi_n^p(\mathbf{r}) = \sum_{m=1}^{d_p} \Gamma(T_p)_{mn}\psi_m^p(\mathbf{r}), \tag{5.12}$$

as $P(T)\psi_n^p(\mathbf{r})$ can be found for each $T \in \mathcal{G}$ using Equation (1.17).

This method will be illustrated by using it to obtain a matrix for the irreducible representation $\mathbf{\Gamma}^5$ of D_4, which is an academic exercise here, as a set is already known.

Example II *Determination of matrix elements of the two-dimensional irreducible representation* $\mathbf{\Gamma}^5$ *of the crystallographic point group* D_4 *from its character system*

Take $\phi(\mathbf{r}) = zF(r)$, where $F(r)$ is any function of r such that $\phi(\mathbf{r})$ is normalized. Then, from Table 4.1 and Equation (5.11), $\mathcal{P}^p\phi(\mathbf{r}) = zF(r)$. As $P(C_{4y}^{-1}\{\mathcal{P}^p\phi(\mathbf{r})\}) = xF(r)$, and as $d_5 = 2$, $zF(r)$ and $xF(r)$ together give the totality of linearly independent functions $P(T)\{\mathcal{P}^p\phi(\mathbf{r})\}$. It happens here that $zF(r)$ and $xF(r)$ are orthogonal, so the Schmidt process is not needed. Then, as $xF(r)$ is also normalized, one may take $\psi_1^5(\mathbf{r}) = zF(r)$ and $\psi_2^5(\mathbf{r}) = xF(r)$. Then, for example,

$$\left.\begin{array}{rcrcl} P(C_{4y})\psi_1^5(\mathbf{r}) & = & -xF(r) & = & -\psi_2^5(\mathbf{r}), \\ P(C_{4y})\psi_2^5(\mathbf{r}) & = & zF(r) & = & \psi_1^5(\mathbf{r}), \end{array}\right\}$$

which, in comparison with Equation (5.12), gives as the matrix representing C_{4y}

$$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}.$$

The matrices representing the other elements of D_4 may be found in the same way. They are not identical to those quoted in Example I above, but could be obtained from them by a similarity transformation (Equation (4.5)) with

$$\mathbf{S} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

2 Direct product representations

In Appendix A, Section 1, the definition is given of the direct product $\mathbf{A} \otimes \mathbf{B}$ of an $m \times m$ matrix $\mathbf{A}$ and an $n \times n$ matrix $\mathbf{B}$ in which $\mathbf{A} \otimes \mathbf{B}$ is an $mn \times mn$ matrix whose rows and columns are each labelled by a pair of indices in such a way that (cf. Equation (A.8))

$$(\mathbf{A} \otimes \mathbf{B})_{js,kt} = A_{jk}B_{st}$$

$(1 \leq j, k \leq m; 1 \leq s, t \leq n)$. Certain properties of direct product matrices are also deduced in that section.

The following theorem shows that this definition allows the construction of "direct product representations", which, through the Wigner-Eckart Theorem, play a major role in the applications of group theory in quantum mechanical problems. (They are sometimes called "Kronecker product representations" or "tensor product representations".)

Theorem I If $\mathbf{\Gamma}^p$ and $\mathbf{\Gamma}^q$ are two unitary irreducible representations of a group $\mathcal{G}$ of dimensions d_p and d_q respectively, then the set of matrices defined by

$$\mathbf{\Gamma}(T) = \mathbf{\Gamma}^p(T) \otimes \mathbf{\Gamma}^q(T) \tag{5.13}$$

for all $T \in \mathcal{G}$ form a unitary representation of $\mathcal{G}$ of dimension $d_p d_q$. The character $\chi(T)$ of $T \in \mathcal{G}$ in this representation is given by

$$\chi(T) = \chi^p(T)\chi^q(T). \tag{5.14}$$

Proof For any T_1 and T_2 of $\mathcal{G}$, by Equation (5.13),

$$\begin{aligned} \mathbf{\Gamma}(T_1)\mathbf{\Gamma}(T_2) &= \{\mathbf{\Gamma}^p(T_1) \otimes \mathbf{\Gamma}^q(T_1)\}\{\mathbf{\Gamma}^p(T_2) \otimes \mathbf{\Gamma}^q(T_2)\} \\ &= \{\mathbf{\Gamma}^p(T_1)\mathbf{\Gamma}^p(T_2)\} \otimes \{\mathbf{\Gamma}^q(T_1)\mathbf{\Gamma}^q(T_2)\} \end{aligned}$$

(on using Equation (A.9)), so

$$\mathbf{\Gamma}(T_1)\mathbf{\Gamma}(T_2) = \mathbf{\Gamma}^p(T_1T_2) \otimes \mathbf{\Gamma}^q(T_1T_2)$$

(as $\mathbf{\Gamma}^p$ and $\mathbf{\Gamma}^q$ are themselves representations), and hence

$$\mathbf{\Gamma}(T_1)\mathbf{\Gamma}(T_2) = \mathbf{\Gamma}(T_1T_2).$$

Thus the matrices $\mathbf{\Gamma}(T)$ of Equation (5.13) certainly form a representation of $\mathcal{G}$ and its dimension is obviously $d_p d_q$. As the direct product of any two unitary matrices is itself unitary (see Appendix A, Section 1), each matrix $\mathbf{\Gamma}(T)$ of Equation (5.13) must be unitary. Finally, as the diagonal elements of $\mathbf{\Gamma}^p(T) \otimes \mathbf{\Gamma}^q(T)$ are labelled by the pairs (j, s) and (k, t) with $j = k$ and $s = t$, for any $T \in \mathcal{G}$

$$\begin{aligned} \chi(T) &= \sum_{j=1}^{d_p}\sum_{s=1}^{d_q}(\mathbf{\Gamma}^p(T) \otimes \mathbf{\Gamma}^q(T))_{js,js} \\ &= \sum_{j=1}^{d_p}\sum_{s=1}^{d_q}\mathbf{\Gamma}^p(T)_{jj}\mathbf{\Gamma}^q(T)_{ss} \\ &= \chi^p(T)\chi^q(T). \end{aligned}$$

The direct product representation defined by Equation (5.13) will be denoted by $\mathbf{\Gamma}^p \otimes \mathbf{\Gamma}^q$. Although its definition in terms of matrix elements of $\mathbf{\Gamma}^p$

and $\mathbf{\Gamma}^q$ may appear complicated, in terms of bases the definition is completely natural, as will be demonstrated in the next two sections.

In general the representation $\mathbf{\Gamma}^p \otimes \mathbf{\Gamma}^q$ is *reducible*, even if $\mathbf{\Gamma}^p$ and $\mathbf{\Gamma}^q$ are themselves irreducible. For example, for the crystallographic point group D_4, as $\mathbf{\Gamma}^5$ is two-dimensional, $\mathbf{\Gamma}^5 \otimes \mathbf{\Gamma}^5$ must be four-dimensional. However, D_4 has no irreducible representations of dimension greater than two, so $\mathbf{\Gamma}^5 \otimes \mathbf{\Gamma}^5$ must be reducible.

Henceforth in this Section it will be assumed that $\mathcal{G}$ is a *finite* group or a *compact* Lie group. Then all the irreducible representations of $\mathcal{G}$ may be assumed to be unitary and every direct product $\mathbf{\Gamma}^p \otimes \mathbf{\Gamma}^q$ is either irreducible or is completely reducible. Suppose that a similarity transformation with a $d_p d_q \times d_p d_q$ non-singular matrix $\mathbf{C}$ is applied to $\mathbf{\Gamma}^p \otimes \mathbf{\Gamma}^q$ to give an equivalent representation that is a direct sum of unitary irreducible representations, and the unitary irreducible representation $\mathbf{\Gamma}^r$ of $\mathcal{G}$ appears n^r_{pq} times in this sum. This can be written formally as

$$\mathbf{\Gamma}^p \otimes \mathbf{\Gamma}^q \approx \sum_r \oplus n^r_{pq} \mathbf{\Gamma}^r, \tag{5.15}$$

or more precisely as

$$\mathbf{C}^{-1}(\mathbf{\Gamma}^p \otimes \mathbf{\Gamma}^q)\mathbf{C} = \sum_r \oplus n^r_{pq} \mathbf{\Gamma}^r, \tag{5.16}$$

where the right-hand side is called the "Clebsch-Gordan series for $\mathbf{\Gamma}^p \otimes \mathbf{\Gamma}^q$". For the case in which $\mathcal{G}$ is a finite group of order g, Theorem V of Chapter 4, Section 6 gives

$$n^r_{pq} = (1/g) \sum_{T \in \mathcal{G}} \chi^p(T) \chi^q(T) \chi^r(T)^*, \tag{5.17}$$

the corresponding expression when $\mathcal{G}$ is a compact Lie group being

$$n^r_{pq} = \int_{\mathcal{G}} \chi^p(T) \chi^q(T) \chi^r(T)^* \, dT. \tag{5.18}$$

Thus in these cases the Clebsch-Gordan series is determined solely by the characters. Obviously, as $\mathbf{\Gamma}^p \otimes \mathbf{\Gamma}^q$ is of dimension $d_p d_q$,

$$d_p d_q = \sum_r n^r_{pq} d_r,$$

where d_r is the dimension of the irreducible representation $\mathbf{\Gamma}^r$.

Example I *Clebsch-Gordan series for the crystallographic point group* D_4
Table 4.1 and Equation (5.17) together imply that

$$\mathbf{\Gamma}^5 \otimes \mathbf{\Gamma}^4 \approx \mathbf{\Gamma}^5$$

(i.e. $n^1_{54} = n^2_{54} = n^3_{54} = n^4_{54} = 0, n^5_{54} = 1$),

$$\mathbf{\Gamma}^5 \otimes \mathbf{\Gamma}^3 \approx \mathbf{\Gamma}^5,$$

and

$$\mathbf{\Gamma}^5 \otimes \mathbf{\Gamma}^5 \approx \mathbf{\Gamma}^1 \oplus \mathbf{\Gamma}^2 \oplus \mathbf{\Gamma}^3 \oplus \mathbf{\Gamma}^4.$$

These particular Clebsch-Gordan series will be needed in later examples. The other series may be found in the same way.

Two useful symmetry properties follow immediately from Equations (5.17) and (5.18), namely

$$n^r_{qp} = n^r_{pq} \tag{5.19}$$

and

$$n^q_{p^* r} = n^r_{pq}, \tag{5.20}$$

where in Equation (5.20) $\mathbf{\Gamma}^{p^*}$ is the irreducible representation of $\mathcal{G}$ defined by $\mathbf{\Gamma}^{p^*}(T) = \{\mathbf{\Gamma}^p(T)\}^*$ for all $T \in \mathcal{G}$, the identity (Equation (5.20)) being a consequence of the fact that n^r_{pq} must be an integer and so must be real.

3 The Wigner-Eckart Theorem for groups of coordinate transformations in $\mathbb{R}^3$

Theorem I Suppose that $\mathcal{G}$ is a group of coordinate transformations in $\mathbb{R}^3$ having irreducible representations $\mathbf{\Gamma}^p$ and $\mathbf{\Gamma}^q$ of dimensions d_p and d_q respectively, and $\phi^p_j(\mathbf{r})$, $j = 1, 2, \ldots, d_p$, and $\psi^q_s(\mathbf{r})$, $s = 1, 2, \ldots, d_q$, are basis functions of $\mathbf{\Gamma}^p$ and $\mathbf{\Gamma}^q$ respectively. Then the set of $d_p d_q$ functions $\phi^p_j(\mathbf{r})\psi^q_s(\mathbf{r})$ (where $j = 1, 2, \ldots, d_p$ and $s = 1, 2, \ldots, d_q$) form a basis for the direct product representation $\mathbf{\Gamma}^p \otimes \mathbf{\Gamma}^q$, provided that they form a linearly independent set.

Proof For any $T \in \mathcal{G}$, from Equation (1.17),

$$\begin{aligned}
P(T)\{\phi^p_j(\mathbf{r})\psi^q_s(\mathbf{r})\} &= \phi^p_j(\{\mathbf{R}(T)|\mathbf{t}(T)\}^{-1}\mathbf{r})\,\psi^q_s(\{\mathbf{R}(T)|\mathbf{t}(T)\}^{-1}\mathbf{r}) \\
&= \{P(T)\phi^p_j(\mathbf{r})\}\{P(T)\psi^q_s(\mathbf{r})\} \\
&= \{\sum_{k=1}^{d_p} \Gamma^p(T)_{kj}\phi^p_k(\mathbf{r})\}\{\sum_{t=1}^{d_q} \Gamma^q(T)_{ts}\phi^q_t(\mathbf{r})\} \\
&= \sum_{k=1}^{d_p}\sum_{t=1}^{d_q} (\mathbf{\Gamma}^p(T) \otimes \mathbf{\Gamma}^q(T))_{kt,js}\,\{\phi^p_k(\mathbf{r})\psi^q_t(\mathbf{r})\},
\end{aligned}$$

which is of the form of Equation (1.26).

Now suppose that $\mathcal{G}$ is a *finite* group or a *compact* Lie group and n^r_{pq} is the number of times that the irreducible representation $\mathbf{\Gamma}^r$ appears in $\mathbf{\Gamma}^p \otimes \mathbf{\Gamma}^q$, where $\mathbf{\Gamma}^p$, $\mathbf{\Gamma}^q$ and $\mathbf{\Gamma}^r$ are all assumed to be unitary. If $n^r_{pq} \neq 0$ there must be n^r_{pq} linearly independent sets of basis functions for $\mathbf{\Gamma}^r$ formed from linear combinations of the products $\phi^p_j(\mathbf{r})\psi^q_s(\mathbf{r})$. Let these be denoted by $\theta^{r,\alpha}_l(\mathbf{r})$,

where $\alpha = 1, 2, \ldots, n^r_{pq}$, and $l = 1, 2, \ldots, d_r$, d_r being the dimension of $\mathbf{\Gamma}^r$, so that

$$P(T)\theta^{r,\alpha}_l(\mathbf{r}) = \sum_{u=1}^{d_r} \Gamma(T)_{ul}\theta^{r,\alpha}_u(\mathbf{r}) \tag{5.21}$$

for all $T \in \mathcal{G}$, $l = 1, 2, \ldots, d_r$, and $\alpha = 1, 2, \ldots, n^r_{pq}$. These may be written in the form

$$\theta^{r,\alpha}_l(\mathbf{r}) = \sum_{j=1}^{d_p}\sum_{k=1}^{d_q} \left(\begin{array}{cc|cc} p & q & r, & \alpha \\ j & k & l & \end{array} \right) \phi^p_j(\mathbf{r})\psi^q_s(\mathbf{r}). \tag{5.22}$$

The coefficients $\left(\begin{array}{cc|cc} p & q & r, & \alpha \\ j & k & l & \end{array} \right)$ are called "Clebsch-Gordan coefficients". They can be regarded as forming a $d_pd_q \times d_pd_q$ non-singular matrix, the rows being labelled by the pairs (j,k), where $j = 1, 2, \ldots, d_p$ and $k = 1, 2, \ldots, d_q$ and the columns being labelled by the triples (r, α, l), where r appears only if $n^r_{pq} \neq 0$, in which case $\alpha = 1, 2, \ldots, n^r_{pq}$ and $l = 1, 2, \ldots, d_r$. In fact this is the matrix $\mathbf{C}$ of Equation (5.16).

The inverse of Equation (5.22) can be written as

$$\phi^p_j(\mathbf{r})\psi^q_s(\mathbf{r}) = \sum_r \sum_{\alpha=1}^{n^r_{pq}} \sum_{l=1}^{d_r} \left(\begin{array}{cc|cc} r, & \alpha & p & q \\ l & & j & k \end{array} \right) \theta^{r,\alpha}_l(\mathbf{r}) \tag{5.23}$$

for all $j = 1, 2, \ldots, d_p$ and $k = 1, 2, \ldots, d_q$, where the sum over r is over all those irreducible representations $\mathbf{\Gamma}^r$ for which $n^r_{pq} \neq 0$. The coefficients $\left(\begin{array}{cc|cc} r, & \alpha & p & q \\ l & & j & k \end{array} \right)$ again form a $d_pd_q \times d_pd_q$ non-singular matrix, but this time the rows are labelled by the triples (r, α, l) and the columns by the pairs (j,k). Clearly this is the matrix $\mathbf{C}^{-1}$ of Equation (5.16).

As $\mathbf{\Gamma}^p \otimes \mathbf{\Gamma}^q$ is unitary and the direct sum on the right-hand side of Equation (5.16) is also unitary, Theorem IV of Chapter 4, Section 3 shows that $\mathbf{C}$ may be chosen to be unitary, which implies that

$$\left(\begin{array}{cc|cc} r, & \alpha & p & q \\ l & & j & k \end{array} \right) = \left(\begin{array}{cc|cc} p & q & r, & \alpha \\ j & k & l & \end{array} \right)^\star. \tag{5.24}$$

Even if the matrix of Clebsch-Gordan coefficients is chosen to be unitary, there is still a degree of arbitrariness in the Clebsch-Gordan coefficients. (See, for example, Chapter 5, Section 3, of Cornwell (1984) for a detailed discussion of this point).

If, for a given pair p and q, $n^r_{pq} \leq 1$ for every r, then it is easy to construct a simple formula for the Clebsch-Gordan coefficients that corresponds to this choice. For a *finite* group $\mathcal{G}$ this is

$$\left(\begin{array}{cc|cc} p & q & r, & \alpha \\ s & t & u & \end{array} \right) = \frac{(d_r/g)^{1/2} \sum_{T\in\mathcal{G}} \Gamma^p(T)_{sj}\Gamma^q(T)_{tk}\Gamma^r(T)^\star_{ul}}{\sum_{T\in\mathcal{G}} \Gamma^p(T)_{jj}\Gamma^q(T)_{kk}\Gamma^r(T)^\star_{ll}}, \tag{5.25}$$

where the set of indices j, k, l are chosen so that the denominator is non-zero. (See Chapter 5, Section 3, of Cornwell (1984) for a proof of this result.)

Although this formula generalizes in the obvious way when $\mathcal{G}$ is a *compact* Lie group, for such a group it is much easier to use Lie algebraic methods to calculate the Clebsch-Gordan coefficients. For example, for SO(3) and SU(2) a description may be found in Chapter 12, Section 5, of Cornwell (1984), the extension for other simple compact Lie groups being given Chapter 16, Section 6, of Cornwell (1984).

When there exists an n_{pq}^{r} such that $n_{pq}^{r} > 1$ the construction of a *unitary* matrix of Clebsch-Gordan coefficients is more difficult and for finite groups there is little advantage in making such a choice. (A detailed discussion may be found in the work of van den Broek and Cornwell (1978).)

The case in which $\mathbf{\Gamma}^{q} = \mathbf{\Gamma}^{1}$, where $\mathbf{\Gamma}^{1}$ is the one-dimensional identity representation defined by $\mathbf{\Gamma}^{1}(T) = [1]$ for all $T \in \mathcal{G}$, provides a simple but important example. In this situation

$$\mathbf{\Gamma}^{p} \otimes \mathbf{\Gamma}^{1} = \mathbf{\Gamma}^{p} \tag{5.26}$$

for every irreducible representation $\mathbf{\Gamma}^{p}$ of $\mathcal{G}$. Moreover Equation (5.25) and its generalization for compact Lie groups, when taken with the orthogonality theorem for matrix representations (Theorem IV of Chapter 4, Section 5), show that the corresponding Clebsch-Gordan coefficients are given by

$$\left(\begin{array}{cc|cc} p & 1 & p, & 1 \\ s & 1 & u & \end{array}\right) = \delta_{su}. \tag{5.27}$$

Example I *Clebsch-Gordan coefficients for the crystallographic point group* D_4

Using the matrices of the two-dimensional irreducible representation $\mathbf{\Gamma}^{5}$ specified in Example I of Section 1, the Clebsch-Gordan coefficients corresponding to the series $\mathbf{\Gamma}^{5} \otimes \mathbf{\Gamma}^{4} \approx \mathbf{\Gamma}^{5}$ are given by Equation (5.25) (with $j = 1$, $k = 1$, $l = 2$) as

$$\left.\begin{array}{l} \left(\begin{array}{cc|cc} 5 & 4 & 5, & 1 \\ 1 & 1 & 2 & \end{array}\right) = \left(\begin{array}{cc|cc} 5 & 4 & 5, & 1 \\ 2 & 1 & 1 & \end{array}\right) = 1, \\ \left(\begin{array}{cc|cc} 5 & 4 & 5, & 1 \\ 1 & 1 & 1 & \end{array}\right) = \left(\begin{array}{cc|cc} 5 & 4 & 5, & 1 \\ 2 & 1 & 2 & \end{array}\right) = 0. \end{array}\right\}$$

Similarly for $\mathbf{\Gamma}^{5} \otimes \mathbf{\Gamma}^{3} \approx \mathbf{\Gamma}^{5}$, Equation (5.25) (with $j = 1$, $k = 1$, $l = 2$) gives

$$\left.\begin{array}{l} \left(\begin{array}{cc|cc} 5 & 3 & 5, & 1 \\ 1 & 1 & 2 & \end{array}\right) = -\left(\begin{array}{cc|cc} 5 & 3 & 5, & 1 \\ 2 & 1 & 1 & \end{array}\right) = 1, \\ \left(\begin{array}{cc|cc} 5 & 3 & 5, & 1 \\ 1 & 1 & 1 & \end{array}\right) = \left(\begin{array}{cc|cc} 5 & 3 & 5, & 1 \\ 2 & 1 & 2 & \end{array}\right) = 0. \end{array}\right\}$$

Likewise, for $\mathbf{\Gamma}^{5} \otimes \mathbf{\Gamma}^{5} \approx \mathbf{\Gamma}^{1} \oplus \mathbf{\Gamma}^{2} \oplus \mathbf{\Gamma}^{3} \oplus \mathbf{\Gamma}^{4}$, Equation (5.25) implies that all

the Clebsch-Gordan coefficients are zero *except* for the following:

$$\left.\begin{array}{rcl}
\left(\begin{array}{cc|cc} 5 & 5 & 1, & 1 \\ 1 & 1 & 1 & \end{array}\right) = \left(\begin{array}{cc|cc} 5 & 5 & 1, & 1 \\ 2 & 2 & 1 & \end{array}\right) = 2^{-1/2}, \\
\left(\begin{array}{cc|cc} 5 & 5 & 2, & 1 \\ 1 & 1 & 1 & \end{array}\right) = -\left(\begin{array}{cc|cc} 5 & 5 & 2, & 1 \\ 2 & 2 & 1 & \end{array}\right) = 2^{-1/2}, \\
\left(\begin{array}{cc|cc} 5 & 5 & 3, & 1 \\ 2 & 1 & 1 & \end{array}\right) = -\left(\begin{array}{cc|cc} 5 & 5 & 3, & 1 \\ 1 & 2 & 1 & \end{array}\right) = 2^{-1/2}, \\
\left(\begin{array}{cc|cc} 5 & 5 & 4, & 1 \\ 2 & 1 & 1 & \end{array}\right) = \left(\begin{array}{cc|cc} 5 & 5 & 4, & 1 \\ 1 & 2 & 1 & \end{array}\right) = 2^{-1/2}.
\end{array}\right\}$$

The Wigner-Eckart Theorem depends on one further concept, that of "irreducible tensor operators".

Definition *Irreducible tensor operators for a group of coordinate transformations in* $\mathbb{R}^3$
Let $Q_1^q, Q_2^q, \ldots$ be a set of d_q linear operators that act on functions belonging to the Hilbert space L^2 and which satisfy the equations

$$P(T)Q_j^q P(T)^{-1} = \sum_{k=1}^{d_q} \Gamma^q(T)_{kj} Q_k^q \tag{5.28}$$

for every $j = 1, 2, \ldots, d_q$ and every T of a group of coordinate transformations $\mathcal{G}$, where $\mathbf{\Gamma}^q$ is an irreducible representation of $\mathcal{G}$ of dimension d_q. Then $Q_1^q, Q_2^q, \ldots$ are said to be a set of "irreducible tensor operators" of the irreducible representation $\mathbf{\Gamma}^q$ of $\mathcal{G}$.

Equations (5.28) are to be interpreted as operator equations, that is, both sides must produce the same result when acting on any function of the common domain in L^2 of the operators Q_j^q. Moreover, on the left-hand side of Equations (5.28), each operator acts on everything to its right.

Example II *The Hamiltonian operator as an irreducible tensor operator*
Let $\mathcal{G}$ be the group of the Schrödinger equation for some system. Then, from Equation (1.23), $P(T)H(\mathbf{r})P(T)^{-1} = H(\mathbf{r})$ for all $T \in \mathcal{G}$. Comparison with Equations (5.28) shows that $H(\mathbf{r})$ is an irreducible tensor operator for the one-dimensional identity representation of the group of the Schrödinger equation.

Example III *Differential operators as irreducible tensor operators of the crystallographic point group* D_4
For any rotation T,

$$\left.\begin{array}{rcl}
P(T)\frac{\partial}{\partial x}P(T)^{-1} &=& R(T)_{11}\frac{\partial}{\partial x} + R(T)_{21}\frac{\partial}{\partial y} + R(T)_{31}\frac{\partial}{\partial z}, \\
P(T)\frac{\partial}{\partial y}P(T)^{-1} &=& R(T)_{12}\frac{\partial}{\partial x} + R(T)_{22}\frac{\partial}{\partial y} + R(T)_{32}\frac{\partial}{\partial z}, \\
P(T)\frac{\partial}{\partial z}P(T)^{-1} &=& R(T)_{13}\frac{\partial}{\partial x} + R(T)_{23}\frac{\partial}{\partial y} + R(T)_{33}\frac{\partial}{\partial z},
\end{array}\right\} \tag{5.29}$$

where $\mathbf{R}(T)$ is the 3×3 orthogonal matrix specifying T.

The first of the Equations (5.29) will now be proved in some detail to illustrate the type of manipulation that is usually involved. For any differential function $f(\mathbf{r})$ of L^2, Equation (1.17) gives

$$P(T)^{-1}f(\mathbf{r}) = P(T^{-1})f(\mathbf{r}) = f(\mathbf{r}'),$$

where $\mathbf{r}' = \mathbf{R}(T)\mathbf{r}$. Thus

$$\begin{aligned} \frac{\partial}{\partial x}\{P(T^{-1})f(\mathbf{r})\} &= \frac{\partial x'}{\partial x}\frac{\partial f(\mathbf{r}')}{\partial x'} + \frac{\partial y'}{\partial x}\frac{\partial f(\mathbf{r}')}{\partial y'} + \frac{\partial z'}{\partial x}\frac{\partial f(\mathbf{r}')}{\partial z'} \\ &= R(T)_{11}\frac{\partial f(\mathbf{r}')}{\partial x'} + R(T)_{21}\frac{\partial f(\mathbf{r}')}{\partial y'} + R(T)_{31}\frac{\partial f(\mathbf{r}')}{\partial z'}, \end{aligned} \tag{5.30}$$

on using Equation (1.2). Now define $h(\mathbf{r}) = \partial f(\mathbf{r})/\partial x$ and put $g(\mathbf{r}) = h(\mathbf{r}')$, where $\mathbf{r}' = \mathbf{R}(T)\mathbf{r}$.. Then, by Equation (1.17),

$$\begin{aligned} P(T)\{\partial f(\mathbf{r}')/\partial x'\} &= P(T)h(\mathbf{r}') = P(T)g(\mathbf{r}) \\ &= g(\mathbf{R}(T)^{-1}\mathbf{r}) = h(\mathbf{r}) = \partial f(\mathbf{r})/\partial x. \end{aligned}$$

A similar argument applied to the second and third terms of Equation (5.30) then gives the first of Equations (5.29) immediately.

Inspection of the matrices $\mathbf{R}(T)$ for D_4 (see Example III of Chapter 1, Section 2) shows that $R(T)_{12} = R(T)_{21} = R(T)_{23} = R(T)_{32} = 0$ for all T of D_4 and $R(T)_{22} = \Gamma^3(T)_{11}$ $(= \chi^3(T))$, where $\mathbf{\Gamma}^3$ is the one-dimensional irreducible representation of D_4 given in the character table, Table 4.1. Thus, from Equations (5.29),

$$P(T)\frac{\partial}{\partial y}P(T)^{-1} = \Gamma^3(T)_{11}\frac{\partial}{\partial y},$$

so that $\partial/\partial y$ is an irreducible tensor operator transforming as $\mathbf{\Gamma}^3$. Inspection also shows that

$$\mathbf{\Gamma}^5(T) = \begin{bmatrix} R(T)_{11} & R(T)_{13} \\ R(T)_{31} & R(T)_{33} \end{bmatrix}$$

for all T of D_4, where $\mathbf{\Gamma}^5$ is the two-dimensional irreducible representation of D_4 (see Example I of Section 1). Thus Equations (5.29) show that Equation (5.28) is satisfied with $q = 5$ and $Q_1^5 = \partial/\partial x$, $Q_2^5 = \partial/\partial z$, so $\partial/\partial x$ and $\partial/\partial z$ constitute a set of irreducible tensor operators for $\mathbf{\Gamma}^5$.

Example IV *Multiplication by a basis function as an irreducible tensor operator*

Let $\psi_j^q(\mathbf{r})$, $j = 1, 2, \ldots, d_q$, be a set of basis functions for the irreducible representation $\mathbf{\Gamma}^q$, and define Q_j^q by

$$Q_j^q f(\mathbf{r}) = \psi_j^q(\mathbf{r})f(\mathbf{r})$$

for $j = 1, 2, \ldots, d_q$, i.e. Q_j^q is the operation of multiplication by $\psi_j^q(\mathbf{r})$. Then $Q_1^q, Q_2^q, \ldots$ form a set of irreducible tensor operators of $\mathbf{\Gamma}^q$, for

$$\begin{aligned} P(T)Q_j^q P(T)^{-1} f(\mathbf{r}) &= P(T)[\psi_j^q(\mathbf{r})\{P(T)^{-1} f(\mathbf{r})\}] \\ &= \{P(T)\psi_j^q(\mathbf{r})\}\{P(T)P(T)^{-1} f(\mathbf{r})\} \\ &= \{\sum_{k=1}^{d_q} \Gamma^q(T)_{kj}\psi_k^q(\mathbf{r})\} f(\mathbf{r}) \\ &= \sum_{k=1}^{d_q} \Gamma^q(T)_{kj} Q_k^q f(\mathbf{r}). \end{aligned}$$

Theorem II *The Wigner-Eckart Theorem for a group of coordinate transformations in* $\mathbb{R}^3$ Let $\mathcal{G}$ be a group of coordinate transformations that is either a *finite* group or a *compact* Lie group. Let $\mathbf{\Gamma}^p$, $\mathbf{\Gamma}^q$ and $\mathbf{\Gamma}^r$ be unitary irreducible representations of $\mathcal{G}$ of dimensions d_p, d_q and d_r respectively, and suppose that $\phi_j^p(\mathbf{r})$, $j = 1, 2, \ldots, d_p$, and $\psi_l^r(\mathbf{r})$, $l = 1, 2, \ldots, d_r$, are sets of basis functions for $\mathbf{\Gamma}^p$ and $\mathbf{\Gamma}^r$ respectively. Finally, let Q_k^q, $k = 1, 2, \ldots, d_q$, be a set of irreducible tensor operators of $\mathbf{\Gamma}^q$. Then

$$(\psi_l^r, Q_k^q \phi_j^p) = \sum_{\alpha=1}^{n_{pq}^r} \left(\begin{array}{cc|cc} p & q & r, & \alpha \\ j & k & l & \end{array} \right)^\star (r|Q^q|p)_\alpha \tag{5.31}$$

for all $j = 1, 2, \ldots, d_p$, $k = 1, 2, \ldots, d_q$, and $l = 1, 2, \ldots, d_r$, where $(r|Q^q|p)_\alpha$ form a set of n_{pq}^r "reduced matrix elements" that are independent of j, k and l.

Proof See, for example, Appendix C, Section 6, of Cornwell (1984). It should be noted that it is not required that the matrix of Clebsch-Gordan coefficients must be unitary.

The Wigner-Eckart Theorem provides both the most succinct and the most powerful expression in the whole field of application of group theory in physical problems. Indeed, most physical applications depend directly on it. It shows that the j, k, l dependence of the quantities $(\psi_l^r, Q_k^q \phi_j^p)$ is given completely by the Clebsch-Gordan coefficients. Moreover, the whole set of $d_p d_q d_r$ elements $(\psi_l^r, Q_k^q \phi_j^p)$ depend only on n_{pq}^r reduced matrix elements.

The theorem has been stated here for the case in which $\mathcal{G}$ is a group of coordinate transformations in $\mathbb{R}^3$ that is either a finite group or a compact Lie group. However, it may be generalized quite easily to any non-compact, semi-simple Lie group, both for the case in which the representations are finite-dimensional (Klimyk 1975) and the case in which they are unitary but infinite-dimensional (Klimyk 1971). Further generalization to unitary representations of non-semi-simple, non-compact Lie groups has also been achieved (Klimyk 1972). See also Agrawala (1980).

The actual definition of the reduced matrix elements is

$$(r|Q^q|p)_\alpha = (1/d_r)\sum_{s=1}^{d_p}\sum_{t=1}^{d_q}\sum_{u=1}^{d_r}\sum_{\alpha=1}^{n^r_{pq}}\left(\begin{array}{cc|cc} p & q & r, & \alpha \\ s & t & u & \end{array}\right)(\psi^r_u, Q^q_t\phi^p_s), \quad (5.32)$$

but in practice the simplest way of determining them is to find n^r_{pq} non-zero elements $(\psi^r_l, Q^q_k\phi^p_j)$ (either by direct evaluation or by fitting to experimental data) and then regard the n^r_{pq} equations (Equations (5.31)) in which these elements appear on the left-hand side as a set of simultaneous equations in $(r|Q^q|p)_\alpha$, $\alpha = 1, 2, \ldots, n^r_{pq}$.

The application of the Wigner-Eckart Theorem to a number of physical problems is described in detail in Chapter 6, particularly in Sections 2 and 3. Frequent use is also made of the following special case.

Theorem III If $\phi^p_j(\mathbf{r})$ (for $j = 1, 2, \ldots, d_p$) and $\psi^q_k(\mathbf{r})$ (for $k = 1, 2, \ldots, d_q$) are respectively basis functions for the unitary irreducible representations $\mathbf{\Gamma}^p$ and $\mathbf{\Gamma}^q$ of the group of the Schrödinger equation $\mathcal{G}$ that is either a *finite* group or a *compact* Lie group, and $\mathbf{\Gamma}^p$ and $\mathbf{\Gamma}^q$ are not equivalent if $p \neq q$ (but are identical if $p = q$), and if $H(\mathbf{r})$ is the Hamiltonian operator, then

$$(\phi^p_m, H\psi^q_n) = 0$$

unless $p = q$ and $m = n$. Moreover, if $p = q$ and $m = n$, then $(\phi^p_m, H\psi^p_m)$ is a constant independent of m.

Proof As noted in Example II above, $H(\mathbf{r})$ is an irreducible tensor operator of the one-dimensional identity representation $\mathbf{\Gamma}^1$ of $\mathcal{G}$. The required result then follows immediately from the Wigner-Eckart Theorem on using Equations (5.26) and (5.27). Alternatively, this theorem may be proved by a simple generalization of the proof of Theorem V of Chapter 4, Section 5, of which it is an obvious extension.

4 The Wigner-Eckart Theorem generalized

It will now be shown how the developments of the previous section can be expressed in terms of the linear operators and carrier spaces first introduced in Chapter 4, Section 1, thereby enabling the theory to apply to any group $\mathcal{G}$ and not merely to groups of coordinate transformations in $\mathbb{R}^3$.

Suppose that the irreducible representations $\mathbf{\Gamma}^p$ and $\mathbf{\Gamma}^q$ of $\mathcal{G}$ have dimensions d_p and d_q and that ψ^p_j (for $j = 1, 2, \ldots, d_p$) and ψ^q_s (for $s = 1, 2, \ldots, d_q$) are ortho-normal bases for the two corresponding abstract inner product spaces V^p and V^q. A $d_p d_q$-dimensional "direct product space" $V^p \otimes V^q$ may be defined as the set of all quantities ϕ of the form

$$\phi = \sum_{j=1}^{d_p}\sum_{s=1}^{d_q} a_{js}\psi^p_j \otimes \psi^q_s,$$

where a_{js} are a set of complex numbers. (This concept is developed in more detail in Appendix B, Section 7.) With an inner product in $V^p \otimes V^q$ defined by

$$(\phi, \psi) = \sum_{j=1}^{d_p} \sum_{s=1}^{d_q} a^*_{js} b_{js},$$

where

$$\psi = \sum_{j=1}^{d_p} \sum_{s=1}^{d_q} b_{js} \psi^p_j \otimes \psi^q_s,$$

the products $\psi^p_j \otimes \psi^q_s$ for $j = 1, 2, \ldots, d_p$, and $s = 1, 2, \ldots, d_q$, form an orthonormal basis for $V^p \otimes V^q$.

Now define the linear operators $\Phi^p(T)$ and $\Phi^q(T)$ for all $T \in \mathcal{G}$ acting on the bases of V^p and V^q respectively by

$$\Phi^p(T)\psi^p_j = \sum_{k=1}^{d_p} \Gamma^p(T)_{kj} \psi^p_k$$

for $j = 1, 2, \ldots, d_p$, and

$$\Phi^q(T)\psi^q_s = \sum_{t=1}^{d_q} \Gamma^q(T)_{ts} \psi^q_t$$

for $s = 1, 2, \ldots, d_q$. These are essentially just Equations (4.1) embellished with extra indices, so $\Phi^p(T)$ and $\Phi^q(T)$ may be extended to the whole of V^p and V^q respectively. For each $T \in \mathcal{G}$, a further linear operator $\Phi(T)$ acting on $V^p \otimes V^q$ may be defined by

$$\Phi(T)\{\psi^p_j \otimes \psi^q_s\} = \{\Phi^p(T)\psi^p_j\} \otimes \{\Phi^q(T)\psi^q_s\} \tag{5.33}$$

and again extended to the whole of V^p and V^q, so that

$$\Phi(T)\{\psi^p_j \otimes \psi^q_s\} = \sum_{k=1}^{d_p} \sum_{t=1}^{d_q} (\mathbf{\Gamma}^p(T) \otimes \mathbf{\Gamma}^q(T))_{kt,js} \{\psi^p_k \otimes \psi^q_t\} \tag{5.34}$$

for all $j = 1, 2, \ldots, d_p$, and $s = 1, 2, \ldots, d_q$. Thus the operators $\Phi(T)$ are the linear operators corresponding to the direct product representation $\mathbf{\Gamma}^p \otimes \mathbf{\Gamma}^q$ of $\mathcal{G}$.

As the Clebsch-Gordan coefficients $\left(\begin{array}{cc|cc} p & q & r, & \alpha \\ j & k & l & \end{array} \right)$ are the matrix elements of a matrix $\mathbf{C}$ that completely reduces $\mathbf{\Gamma}^p \otimes \mathbf{\Gamma}^q$ (see Equation (5.16)), it follows that for $n^r_{pq} \neq 0$ the elements of $V^p \otimes V^q$ defined by

$$\theta^{r,\alpha}_l = \sum_{j=1}^{d_p} \sum_{k=1}^{d_q} \left(\begin{array}{cc|cc} p & q & r, & \alpha \\ j & k & l & \end{array} \right) \psi^p_j \otimes \psi^q_k \tag{5.35}$$

satisfy

$$\Phi(T)\theta_l^{r,\alpha} = \sum_{u=1}^{d_r} \Gamma^r(T)_{ul}\theta_u^{r,\alpha} \tag{5.36}$$

for all $T \in \mathcal{G}$, $l = 1, 2, \ldots, d_r$ and $\alpha = 1, 2, \ldots, n_{pq}^r$. That is, again the Clebsch-Gordan coefficients give the appropriate linear combinations that form bases for the various irreducible representations of $\mathbf{\Gamma}^p \otimes \mathbf{\Gamma}^q$, the similarities between Equations (5.35) and (5.22) and between Equations (5.36) and (5.21) being particularly significant.

(In comparing the developments of this section with those of Section 3, it must be observed that the products $\phi_j^p(\mathbf{r})\psi_s^q(\mathbf{r})$ of the basis functions $\phi_j^p(\mathbf{r})$ of $\mathbf{\Gamma}^p$ and $\psi_s^q(\mathbf{r})$ of $\mathbf{\Gamma}^q$ form a basis for a $d_p d_q$-dimensional subspace of L^2 *only* if they are linearly independent, and even then these products do *not* necessarily form an ortho-normal set with respect to the usual inner product of L^2. By contrast, the products $\psi_j^p \otimes \psi_s^q$ of basis vectors ψ_j^p and ψ_s^q of V^p and V_q *always* form an ortho-normal basis of $V^p \otimes V_q$ with the inner product defined as above. Thus for basis functions in general one *cannot* identify $\phi_j^p(\mathbf{r}) \otimes \psi_s^q(\mathbf{r})$ with $\phi_j^p(\mathbf{r})\psi_s^q(\mathbf{r})$ and at the same time take the inner product of $V^p \otimes V_q$ to be that of L^2.)

To proceed further it is necessary to redefine the concept of a set of irreducible tensor operators. To this end let Q be a linear mapping of V^p into V^r (V^p and V^r being carrier spaces for the irreducible representations $\mathbf{\Gamma}^p$ and $\mathbf{\Gamma}^r$ of $\mathcal{G}$) so that $Q\psi \in V^r$ for all $\psi \in V^p$. Defining the sum $(Q_1 + Q_2)$ of two such operators Q_1 and Q_2 by $(Q_1 + Q_2)\psi = Q_1\psi + Q_2\psi$ (for all $\psi \in V^p$), the product aQ for any complex number a by $(aQ)\psi = a(Q\psi)$ (for all $\psi \in V^p$), and the "zero" mapping 0 by $0\psi = 0$ (for all $\psi \in V^p$, where the 0 on the right-hand side here is the "zero" element of V^r), it follows that the set of all linear mappings Q from V^p to V^r form a vector space. which will be denoted by $L(V^p, V^r)$. If V^p and V^r are of dimensions d_p and d_r respectively, then $L(V^p, V^r)$ is of dimension $d_p d_r$ (Shephard 1966).

Now define for each $T \in \mathcal{G}$ an operator $\Phi'(T)$ acting on $L(V^p, V^r)$ by

$$\Phi'(T)Q = \Phi^r(T)\, Q\, \Phi^p(T)^{-1}$$

for all $Q \in L(V^p, V^r)$, $\Phi^p(T)$ and $\Phi^r(T)$ being the operators acting in V^p and V^r belonging (in the manner described above) to the irreducible representations $\mathbf{\Gamma}^p$ and $\mathbf{\Gamma}^r$. Then $\Phi'(T)$ is a linear operator, and for any $T_1, T_2 \in \mathcal{G}$

$$\Phi'(T_1)\Phi'(T_2) = \Phi'(T_1T_2),$$

so that the set of operators $\Phi'(T)$ correspond to a representation of $\mathcal{G}$ for which the carrier space is $L(V^p, V^r)$. (The proof of this statement is as follows. For any $T_1, T_2 \in \mathcal{G}$ and any $Q \in L(V^p, V^r)$,

$$\begin{aligned}
\Phi'(T_1)\Phi'(T_2)Q &= \Phi^r(T_1)\{\Phi^r(T_2)\, Q\, \Phi^p(T_2)^{-1}\}\Phi^p(T_1)^{-1} \\
&= \Phi^r(T_1T_2)\, Q\, \Phi^p(T_1T_2)^{-1} \\
&= \Phi'(T_1T_2)Q.)
\end{aligned}$$

Let $\mathbf{\Gamma}'$ be the representation of $\mathcal{G}$ for which the operators $\Phi'(T)$ and the carrier space $L(V^p, V^r)$ form a module. That is, if $Q_1, Q_2, \ldots$ are a basis of the vector space $L(V^p, V^r)$, the matrix elements $\Gamma'(T)_{mn}$ are defined by

$$\Phi'(T)Q_n = \sum_{m=1}^{d_p d_r} \Gamma'(T)_{mn} Q_m$$

for all $T \in \mathcal{G}$. In general $\mathbf{\Gamma}'$ is reducible. Suppose that $\mathbf{\Gamma}'$ is completely reducible and that $\mathbf{\Gamma}^q$ is an irreducible representation that appears in its reduction, and let $Q_1^q, Q_2^q, \ldots$ be a basis for the corresponding subspace of $L(V^p, V^r)$. Then

$$\Phi'(T)Q_n^q = \sum_{m=1}^{d_q} \Gamma^q(T)_{mn} Q_m^q$$

for $n = 1, 2, \ldots, d_q$ and all $T \in \mathcal{G}$. That is, by the definition of $\Phi'(T)$,

$$\Phi^r(T)\, Q_n^q\, \Phi^p(T)^{-1} = \sum_{m=1}^{d_q} \Gamma^q(T)_{mn} Q_m^q \tag{5.37}$$

for $n = 1, 2, \ldots, d_q$, and all $T \in \mathcal{G}$. This set of operators will be called "irreducible tensor operators of the irreducible representation $\mathbf{\Gamma}^q$ of $\mathcal{G}$".

Theorem I *The generalized Wigner-Eckart Theorem* Let $\mathcal{G}$ be a finite group or a compact Lie group. Let $\mathbf{\Gamma}^p$, $\mathbf{\Gamma}^q$ and $\mathbf{\Gamma}^r$ be unitary irreducible representations of $\mathcal{G}$ of dimensions d_p, d_q and d_r respectively, and suppose that ϕ_j^p $(j = 1, 2, \ldots, d_p)$ and ψ_l^r $(l = 1, 2, \ldots, d_r)$ are basis vectors of orthonormal bases of the carrier spaces V^p and V^r of $\mathbf{\Gamma}^p$ and $\mathbf{\Gamma}^r$ respectively. Finally, let Q_k^q $(k = 1, 2, \ldots, d_q)$ be a set of irreducible tensor operators of $\mathbf{\Gamma}^q$, defined as above. Then

$$(\psi_l^r, Q_k^q \phi_j^p) = \sum_{\alpha=1}^{n_{pq}^r} \left(\begin{array}{cc|cc} p & q & r, & \alpha \\ j & k & l & \end{array} \right)^{\star} (r|Q^q|p)_\alpha \tag{5.38}$$

for all $j = 1, 2, \ldots, d_p$, $k = 1, 2, \ldots, d_q$ and $l = 1, 2, \ldots, d_r$, where $(r|Q^q|p)_\alpha$ are a set of n_{pq}^r "reduced matrix elements" that are independent of j, k and l.

Proof See, for example, Chapter 5, Section 4, and Appendix C, Section 6, of Cornwell (1984).

It should be noted that the appropriate inner product on the left-hand side of Equation (5.38) is that of V^r, as ψ_l^r and $Q_k^q \phi_j^p$ are both members of V^r. The remarks made in Section 3 about the Wigner-Eckart Theorem for a group of transformations in $\mathbb{R}^3$ apply equally to the theorem as generalized above. In particular, although the theorem is stated and proved here for the case in which $\mathcal{G}$ is a finite group or compact Lie group, the conclusion is valid

much more generally. A detailed discussion of the range of validity has been given by Agrawala (1980).

In a minor extension of this formalism, one could introduce an inner product space V that is a direct sum of carrier spaces of certain unitary irreducible representations of $\mathcal{G}$ and which contains at least $V^p \oplus V^r$ (and which, in the extreme case, may contain one carrier space for every inequivalent irreducible representation of $\mathcal{G}$). Then, for each $T \in \mathcal{G}$ an operator $\Phi(T)$ can be defined which maps elements of V into V, and which acts as $\Phi^p(T)$ on V^p, as $\Phi^r(T)$ on V^r, and so on. The irreducible tensor operators are then required to each map V into V and to be such that $\Phi(T)\, Q_n^q\, \Phi(T)^{-1} = \sum_{m=1}^{d_q} \Gamma^q(T)_{mn} Q_m^q$ for all $T \in \mathcal{G}$ and all $n = 1, 2, \ldots, d_q$. In this case the Wigner-Eckart theorem deals with inner products defined on V, but is otherwise the same as above.

5 Representations of direct product groups

The concept of direct product groups was discussed in some detail in Chapter 2, Section 7. In studies of their representations it is most convenient (and quite sufficient) to revert to the original formulation in terms of pairs.

Theorem I Let $\mathbf{\Gamma}_1$ and $\mathbf{\Gamma}_2$ be representations of $\mathcal{G}_1$ and $\mathcal{G}_2$ respectively. Then the set of matrices $\mathbf{\Gamma}((T_1, T_2))$ defined for all $T_1 \in \mathcal{G}_1$ and $T_2 \in \mathcal{G}_2$ by

$$\mathbf{\Gamma}((T_1, T_2)) = \mathbf{\Gamma}_1(T_1) \otimes \mathbf{\Gamma}_2(T_2) \tag{5.39}$$

provides a representation of $\mathcal{G}_1 \otimes \mathcal{G}_2$. This representation of $\mathcal{G}_1 \otimes \mathcal{G}_2$ is unitary if $\mathbf{\Gamma}_1$ and $\mathbf{\Gamma}_2$ are unitary representations and is faithful if $\mathbf{\Gamma}_1$ and $\mathbf{\Gamma}_2$ are faithful representations.

Proof For any $T_1, T_1' \in \mathcal{G}_1$ and any $T_2, T_2' \in \mathcal{G}_2$, from Equation (5.39),

$$\begin{aligned} \mathbf{\Gamma}((T_1, T_2))\mathbf{\Gamma}((T_1', T_2')) &= \{\mathbf{\Gamma}_1(T_1) \otimes \mathbf{\Gamma}_2(T_2)\}\{\mathbf{\Gamma}_1(T_1') \otimes \mathbf{\Gamma}_2(T_2')\} \\ &= \{\mathbf{\Gamma}_1(T_1)\mathbf{\Gamma}_1(T_1')\} \otimes \{\mathbf{\Gamma}_2(T_2)\mathbf{\Gamma}_2(T_2')\} \end{aligned}$$

(on using Equation (A.9)), so

$$\mathbf{\Gamma}((T_1, T_2))\mathbf{\Gamma}((T_1', T_2')) = \mathbf{\Gamma}_1(T_1 T_1') \otimes \mathbf{\Gamma}_2(T_2 T_2'),$$

(as $\mathbf{\Gamma}_1$ and $\mathbf{\Gamma}_2$ are assumed representations of $\mathcal{G}_1$ and $\mathcal{G}_2$ respectively), and hence

$$\begin{aligned} \mathbf{\Gamma}((T_1, T_2))\mathbf{\Gamma}((T_1', T_2')) &= \mathbf{\Gamma}((T_1 T_1', T_2 T_2')) \\ &= \mathbf{\Gamma}((T_1, T_2), (T_1' T_2')) \end{aligned}$$

(on using Equation (2.11)). Consequently the matrices $\mathbf{\Gamma}$ of Equation (5.39) form a representation of $\mathcal{G}_1 \otimes \mathcal{G}_2$. The unitary property follows from the fact that the direct product of two unitary matrices is itself unitary (see Appendix A, Section 1), while the faithful property is obvious.

This theorem allows the nature of $\mathcal{G}_1 \otimes \mathcal{G}_2$ to be investigated when $\mathcal{G}_1$ and $\mathcal{G}_2$ are finite groups or linear Lie groups. There are essentially three distinct cases:

(i) *$\mathcal{G}_1$ and $\mathcal{G}_2$ are both finite groups.*
In this case clearly $\mathcal{G}_1 \otimes \mathcal{G}_2$ is a finite group whose order is the product of those of $\mathcal{G}_1$ and $\mathcal{G}_2$ separately.

(ii) *$\mathcal{G}_1$ is a finite group and $\mathcal{G}_2$ is a linear Lie group.*
Suppose that $\mathcal{G}_1$ has order g_1 and has a faithful finite-dimensional representation $\mathbf{\Gamma}_1$. Suppose that $\mathcal{G}_2$ has a faithful finite-dimensional representation $\mathbf{\Gamma}_2$, that the elements of $\mathcal{G}_2$ near the identity are specified by n real parameters $x_1, x_2, \ldots, x_n$, and that $\mathcal{G}_2$ has N connected components. Then the faithful finite-dimensional representation of Equation (5.39) can be used to show that $\mathcal{G}_1 \otimes \mathcal{G}_2$ is a linear Lie group with Ng_1 connected components, whose connected subgroup is isomorphic to the set of matrices $\mathbf{\Gamma}_1(E_1) \otimes \mathbf{\Gamma}_2(T_2)$ for all T_2 of the connected subgroup of $\mathcal{G}_2$. Moreover, the elements of $\mathcal{G}_1 \otimes \mathcal{G}_2$ near the identity of $\mathcal{G}_1 \otimes \mathcal{G}_2$ may be specified by the same n real parameters as for $\mathcal{G}_2$. As the "invariant integral" of $\mathcal{G}_1 \otimes \mathcal{G}_2$ involves an integral over n variables with the same weight function as for $\mathcal{G}_2$ and a sum over the Ng_1 connected components, it is obvious that $\mathcal{G}_1 \otimes \mathcal{G}_2$ is compact if and only if $\mathcal{G}_2$ is compact.

(iii) *$\mathcal{G}_2$ is a finite group and $\mathcal{G}_1$ is a linear Lie group.*
This is just the same as the previous case with the roles of $\mathcal{G}_1$ and $\mathcal{G}_2$ interchanged.

(iv) *$\mathcal{G}_1$ and $\mathcal{G}_2$ are both linear Lie groups.*
Suppose that $\mathbf{\Gamma}_j$ is a faithful finite-dimensional representation of $\mathcal{G}_j$, that the elements of $\mathcal{G}_j$ near the identity of $\mathcal{G}_j$ are specified by n_j real parameters, and that $\mathcal{G}_j$ has N_j components ($j = 1, 2$). Then the faithful finite-dimensional representation (Equation (5.39)) of $\mathcal{G}_1 \otimes \mathcal{G}_2$ can be employed to prove that $\mathcal{G}_1 \otimes \mathcal{G}_2$ is a linear Lie group with $N_1 N_2$ connected components and that the elements of $\mathcal{G}_1 \otimes \mathcal{G}_2$ near the identity of $\mathcal{G}_1 \otimes \mathcal{G}_2$ are specified by $(n_1 + n_2)$ real parameters. The "invariant integral" of $\mathcal{G}_1 \otimes \mathcal{G}_2$ therefore involves an integral over $(n_1 + n_2)$ variables (whose weight function is the product of those of $\mathcal{G}_1$ and $\mathcal{G}_2$ separately) and a sum over the $N_1 N_2$ components, so that $\mathcal{G}_1 \otimes \mathcal{G}_2$ is compact if and only if $\mathcal{G}_1$ and $\mathcal{G}_2$ are both compact.

Theorem II If $\mathcal{G}_1 \otimes \mathcal{G}_2$ is a finite group or a compact linear Lie group and $\mathbf{\Gamma}_1$ and $\mathbf{\Gamma}_2$ are irreducible representations of $\mathcal{G}_1$ and $\mathcal{G}_2$ respectively, then the representation $\mathbf{\Gamma}$ defined by Equation (5.39) is an *irreducible* representation of $\mathcal{G}_1 \otimes \mathcal{G}_2$. Moreover, *every* irreducible representation of $\mathcal{G}_1 \otimes \mathcal{G}_2$ is equivalent to a representation constructed in this way.

Proof See, for example, Appendix C, Section 7, of Cornwell (1984).

6 Irreducible representations of finite Abelian groups

The irreducible representations of every *finite Abelian* group $\mathcal{G}$ may now be found very easily. It should be recalled that Theorem III of Chapter 4, Section 5 shows that these representations must be one-dimensional, and as every representation of a finite group is equivalent to a unitary representation (equivalence implying identity for one-dimensional representations), all these irreducible representations are automatically unitary. Moreover, Theorem VIII of Chapter 4, Section 6 and Theorem II of Chapter 2, Section 2 together imply that the number of inequivalent irreducible representations of $\mathcal{G}$ is equal to the order of $\mathcal{G}$.

The first stage is to consider a special type of Abelian group.

Definition *Cyclic group*
A group is said to be "cyclic" if every element can be expressed as a power of a single element.

The most general form of a finite cyclic group of order g is therefore $\{E, T, T^2, \ldots, T^{g-1}\}$, with $T^g = E$, the element T being called the "generator" of $\mathcal{G}$. Obviously every cyclic group is Abelian. It is easily shown that all cyclic groups of the same order are isomorphic.

Theorem I The set of all unitary irreducible representations of a cyclic group of order g is given by

$$\mathbf{\Gamma}^p(T^m) = [\exp\{2\pi i m(p-1)/g\}] \tag{5.40}$$

for $m = 1, 2, \ldots, g$. Here p takes values $p = 1, 2, \ldots, g$, and T is the generator of $\mathcal{G}$.

Proof Suppose that $\mathbf{\Gamma}$ is an irreducible representation and $\mathbf{\Gamma}(T) = [\gamma]$, where γ is some complex number. Then $\gamma^g = 1$ as $T^g = E$, so γ can take any of the g possible values $\gamma = \exp\{2\pi i(p-1)/g\}$, where $p = 1, 2, \ldots, g$. These g values of γ then give the g inequivalent irreducible representations, which may therefore be labelled by p. As $\mathbf{\Gamma}^p(T^m) = \{\mathbf{\Gamma}^p(T)\}^m = [\gamma^m]$, Equation (5.40) follows immediately.

The factor $\exp\{2\pi i m(p-1)/g\}$ has been introduced in Equation (5.40) instead of the factor $\exp\{2\pi i m p/g\}$ simply to ensure conformity with the usual convention that $\mathbf{\Gamma}^1$ is the identity representation.

The following theorem shows that any finite Abelian group is made up of cyclic groups and so enables all its irreducible representations to be calculated immediately.

Theorem II Every finite Abelian group is either a finite cyclic group or is isomorphic to a direct product of a set of finite cyclic groups.

Proof See, for example, Rotman (1965) (pages 58 to 62).

Example I *Irreducible representations of groups isomorphic to $C_r \otimes C_s$, C_r and C_s being cyclic groups of order r and s respectively*
Let Γ_1^p be an irreducible representation of C_r, so that, by Equation (5.40), $\Gamma_1^p({T_1}^m) = [\exp\{2\pi i m(p-1)/r\}]$, where T_1 is the generator of C_r. Similarly, let Γ_2^q be an irreducible representation of C_s, with generator T_2, so that $\Gamma_2^q({T_2}^n) = [\exp\{2\pi i n(q-1)/s\}]$. Then, by the theorems of the previous section, the irreducible representations of every group isomorphic to $C_r \otimes C_s$ may be labelled by a pair (p,q), where $p = 1,2,\ldots,r$, and $q = 1,2,\ldots,s$, and, from Equation (5.39),

$$\Gamma^{p,q}(({T_1}^m,{T_2}^n)) = [\exp\{2\pi i(\{m(p-1)/r\} + \{n(q-1)/s\})\}]$$

for all $m = 1,2,\ldots,r$ and $n = 1,2,\ldots,s$.

The crystallographic point group D_2 (see Appendix C) is an example having this structure, as it is isomorphic to $C_2 \otimes C_2$.

7 Induced representations

The method of "induction" provides a very powerful technique for constructing representations of a group from representations of its subgroups. It will be described here for the case in which the group is finite and the results obtained will be applied in Chapter 7 to the symmorphic crystallographic space groups. However, the technique is not restricted to finite groups. Indeed, one of the most significant developments of the last few years has been the generalization to arbitrary, locally compact topological groups, including particularly Lie groups. This development has been largely pioneered by the work of Mackey (1963, 1968, 1976). It has proved extremely valuable in the construction of the infinite-dimensional unitary representations of noncompact, semi-simple Lie groups (Stein 1965, Lipsman 1974, Barut and Raczka 1977), thereby putting into a general context the original work on the homogeneous Lorentz group (Gel'fand *et al.* 1963, Naimark 1957, 1964). Other physically important non-compact Lie groups that are particularly well suited to treatment by the induced representation method include the Poincaré group (Wigner 1939, Bertrand 1966, Halpern 1968, Niederer and O'Raifeartaigh 1974a,b), the Galilei group (Inönü and Wigner 1952, Voisin 1965a,b, 1966, Brennich 1970, Niederer and O'Raifeartaigh 1974a) and the Euclidean group of $\mathbb{R}^3$ (Miller 1964, Niederer and O'Raifeartaigh 1974a).

Most of the results to be derived in this section for finite groups carry over to the general case of locally compact topological groups with their group theoretical content essentially unchanged. The complications of the general case lie in the measure theoretic questions involved, together with the fact that nearly all the representations that appear are infinite-dimensional. Coleman (1968) has given a very readable introduction to these matters.

The basic theorem on induced representation is easily stated and proved:

Theorem I Let $\mathcal{S}$ be a subgroup, of order s, of a group $\mathcal{G}$ of order g, and let $T_1, T_2, \ldots$ be a set of $M(= g/s)$ coset representatives for the decomposition of $\mathcal{G}$ into right cosets with respect to $\mathcal{S}$. Let $\mathbf{\Delta}$ be a d-dimensional unitary representation of $\mathcal{S}$. Then the set of $Md \times Md$ matrices $\mathbf{\Gamma}(T)$, defined for all $T \in \mathcal{G}$ by

$$\Gamma(T)_{kt,jr} = \begin{cases} \Delta(T_k T T_j^{-1})_{tr}, & \text{if } T_k T T_j^{-1} \in \mathcal{S}, \\ 0, & \text{if } T_k T T_j^{-1} \notin \mathcal{S}, \end{cases} \tag{5.41}$$

provides an Md-dimensional unitary representation of $\mathcal{G}$. If $\psi(S)$ are the characters of the representation $\mathbf{\Delta}$ of $\mathcal{S}$, then the characters $\chi(T)$ of the representation $\mathbf{\Gamma}$ of $\mathcal{G}$ are given by

$$\chi(T) = \sum_j \psi(T_j T T_j^{-1}), \tag{5.42}$$

where the sum is over all coset representatives T_j such that $T_j T T_j^{-1} \in \mathcal{S}$.

Proof See, for example, Appendix C, Section 8, of Cornwell (1984).

This representation $\mathbf{\Gamma}$ of $\mathcal{G}$ is said to be "induced" from the representation $\mathbf{\Delta}$ of the subgroup $\mathcal{S}$, this being indicated by writing

$$\mathbf{\Gamma} = \mathbf{\Delta}(\mathcal{S}) \uparrow \mathcal{G}.$$

In Equations (5.41) the rows and the columns of $\mathbf{\Gamma}(T)$ are each separately labelled by a *pair* of indices, exactly as in the theory of direct product representations (see Section 2 and Appendix A, Section 1). The theorem (and proof) is also valid when $\mathcal{G}$ and $\mathcal{S}$ are compact Lie groups such that the decomposition of $\mathcal{G}$ into right cosets with respect to $\mathcal{S}$ contains only a *finite* number M of distinct cosets.

For one physically important type of group the induced representation method not only produces irreducible representations of the group, but it generates the *whole* set of such representations. This satisfactory situation occurs when $\mathcal{G}$ has the *semi-direct product* structure $\mathcal{A} \circledS \mathcal{B}$ and the invariant subgroup $\mathcal{A}$ is *Abelian* (see Chapter 2, Section 7). Physically important groups with this structure include the Euclidean group of $\mathbb{R}^3$ (see Example II of Chapter 2, Section 7), the Poincaré group, and the symmorphic crystallographic space groups (see Chapter 7). Of these only the latter are finite but all the results to be described can be generalized easily to the other groups. The construction of the unitary irreducible representations of $\mathcal{G}$ involves a number of stages which will now be described in detail. It will be assumed that the orders of $\mathcal{G}$, $\mathcal{A}$ and $\mathcal{B}$ are g, a and b respectively, so that $g = ab$.

(a) As $\mathcal{A}$ is Abelian it possesses a inequivalent irreducible representations, all of which are one-dimensional and therefore completely specified by their characters. Let these characters be denoted by $\chi_{\mathcal{A}}^q(A)$, $q = 1, 2, \ldots, a$, for all $A \in \mathcal{A}$.

(b) Let $\mathcal{B}(q)$ be the subset of elements B of $\mathcal{B}$ such that

$$\chi^q_{\mathcal{A}}(BAB^{-1}) = \chi^q_{\mathcal{A}}(A) \tag{5.43}$$

for all $A \in \mathcal{A}$. Then $\mathcal{B}(q)$ is a subgroup of $\mathcal{B}$. $\mathcal{B}(q)$ is called a "little group". (As $\mathcal{A}$ is an invariant subgroup of $\mathcal{G}$, $BAB^{-1} \in \mathcal{A}$ for all $A \in \mathcal{A}$ and all $B \in \mathcal{B}$, so $\mathcal{B}(q)$ is well defined. The subgroup property follows because, if B and B' are members of $\mathcal{B}(q)$, then for any $A \in \mathcal{A}$, from Equation (5.43),

$$\chi^q_{\mathcal{A}}((B'B^{-1})A(B'B^{-1})^{-1}) = \chi^q_{\mathcal{A}}(B^{-1}AB) = \chi^q_{\mathcal{A}}(A),$$

so that $B'B^{-1}$ is also a member of $\mathcal{B}(q)$.) Let $b(q)$ be the order of $\mathcal{B}(q)$.

(c) Let $B_1, B_2, \ldots$ be the set of $M(q)(= b/b(q))$ coset representatives for the decomposition of $\mathcal{B}$ into right cosets with respect to $\mathcal{B}(q)$.

(d) For each $B \in \mathcal{B}$ define the quantities $\chi^{B(q)}_{\mathcal{A}}(A)$ for all $A \in \mathcal{A}$ by

$$\chi^{B(q)}_{\mathcal{A}}(A) = \chi^q_{\mathcal{A}}(BAB^{-1}). \tag{5.44}$$

Then, for each fixed B, the set $\chi^{B(q)}_{\mathcal{A}}(A)$ is a set of characters of a one-dimensional irreducible representation of $\mathcal{A}$, so that $B(q)$ is an integer in the set $1, 2, \ldots, a$. That $\chi^{B(q)}_{\mathcal{A}}(A)$ are such characters can be demonstrated as follows. Let A and A' be any two elements of $\mathcal{A}$. Then

$$\begin{aligned}
\chi^{B(q)}_{\mathcal{A}}(A)\chi^{B(q)}_{\mathcal{A}}(A') &= \chi^q_{\mathcal{A}}(BAB^{-1})\chi^q_{\mathcal{A}}(BA'B^{-1}) \\
&= \chi^q_{\mathcal{A}}((BAB^{-1})(BA'B^{-1})) \\
&= \chi^q_{\mathcal{A}}(B(AA')B^{-1}) \\
&= \chi^{B(q)}_{\mathcal{A}}(AA').
\end{aligned}$$

(e) Obviously Equations (5.43) and (5.44) imply that $B(q) = q$ for all $B \in \mathcal{B}(q)$. More generally, $B(q) = B_j(q)$ for every $B \in \mathcal{B}$ belonging to the right coset $\mathcal{B}(q)B_j$. This follows because if $B \in \mathcal{B}(q)B_j$ then there exists an element B' of $\mathcal{B}(q)$ such that $B = B'B_j$. Then for any $A \in \mathcal{A}$

$$\begin{aligned}
\chi^{B(q)}_{\mathcal{A}}(A) &= \chi^q_{\mathcal{A}}((B'B_j)A(B'B_j)^{-1}) && \text{(by Equation (5.44))} \\
&= \chi^q_{\mathcal{A}}(B_jAB_j^{-1}) && \text{(by Equation (5.43))} \\
&= \chi^{B_j(q)}_{\mathcal{A}}(A) && \text{(by Equation (5.44)).}
\end{aligned}$$

(f) The set of $M(q)(= b/b(q))$ integers $\{B_1(q)(= q), B_2(q), B_3(q), \ldots\}$ is known as the "orbit" of q.

(g) The groups $\mathcal{B}(B_j(q))$ are all isomorphic to $\mathcal{B}(q)$ for $j = 1, 2, \ldots, M(q)$. That is, all members of the orbit of q are associated with essentially

the same group $\mathcal{B}(q)$. (Equation (5.43) implies that $\mathcal{B}(B_j(q))$ is the subgroup of $\mathcal{B}$ consisting of all $B \in \mathcal{B}$ such that

$$\chi_{\mathcal{A}}^{B_j(q)}(BAB^{-1}) = \chi_{\mathcal{A}}^{B_j(q)}(A)$$

for all $A \in \mathcal{A}$. By Equation (5.44) this can be rewritten as

$$\chi_{\mathcal{A}}^{q}(B_jBAB^{-1}B_j^{-1}) = \chi_{\mathcal{A}}^{q}(B_jAB_j^{-1}) \tag{5.45}$$

for all $A \in \mathcal{A}$. Now consider the automorphic mapping ϕ_j of $\mathcal{G}$ onto itself defined by $\phi_j(T) = B_jTB_j^{-1}$. As $\mathcal{A}$ is an invariant subgroup of $\mathcal{G}$, this provides a one-to-one mapping of $\mathcal{A}$ onto itself. Consequently, let A' be any element of $\mathcal{A}$ and let $A = B_j^{-1}A'B_j$. Then Equation (5.45) can be further rewritten as

$$\chi_{\mathcal{A}}^{q}((B_jBB_j^{-1})A'(B_jBB_j^{-1})^{-1}) = \chi_{\mathcal{A}}^{q}(A')$$

for all $A' \in \mathcal{A}$. Thus $\phi_j(B) = B_jBB_j^{-1}$ maps $\mathcal{B}(B_j(q))$ onto $\mathcal{B}(q)$ and, as ϕ_j is an isomorphic mapping, $\mathcal{B}(q)$ is isomorphic to $\mathcal{B}(B_j(q))$.)

(h) Let $\mathcal{S}(q)$ be the set of all products AB, where $A \in \mathcal{A}$ and $B \in \mathcal{B}(q)$. Then $\mathcal{S}(q)$ is a subgroup of $\mathcal{G}$ with the semi-direct product structure $\mathcal{A}\circledS\,\mathcal{B}(q)$. (If $A, A' \in \mathcal{A}$ and $B, B' \in \mathcal{B}(q)$, then, as $\mathcal{A}$ is an invariant subgroup of $\mathcal{G}$, there exists an $A'' \in \mathcal{A}$ such that $(B'B^{-1})A^{-1} = A''(B'B^{-1})$. Consequently

$$(A'B')(AB)^{-1} = A'B'B^{-1}A^{-1} = AA''B'B^{-1},$$

which is a member of $\mathcal{S}(q)$, as $AA'' \in \mathcal{A}$ and $B'B^{-1} \in \mathcal{B}(q)$. The semi-direct product structure of $\mathcal{S}(q)$ follows directly from that of $\mathcal{G}$.)

(i) Let $\mathbf{\Gamma}^p_{\mathcal{B}(q)}$ be a unitary irreducible representation of $\mathcal{B}(q)$ of dimension d_p. Then the set of $d_p \times d_p$ matrices $\mathbf{\Delta}^{q,p}(AB)$ defined by

$$\mathbf{\Delta}^{q,p}(AB) = \chi_{\mathcal{A}}^{q}(A)\mathbf{\Gamma}^p_{\mathcal{B}(q)}(B) \tag{5.46}$$

for all $A \in \mathcal{A}$ and $B \in \mathcal{B}(q)$ form a d_p-dimensional unitary representation of $\mathcal{S}(q)$. (That $\mathbf{\Delta}^{q,p}$ is a representation $\mathcal{S}(q)$ can be proved as follows. Let A, A' be any two elements of $\mathcal{A}$ and B, B' any two elements of $\mathcal{B}(q)$. Then there exists an $A'' \in \mathcal{A}$ such that $BA'B^{-1} = A''$, so, from Equation (5.43), $\chi^p(A') = \chi^q(A'')$. Thus, from Equation (5.46),

$$\begin{aligned}
\mathbf{\Delta}^{q,p}((AB)(A'B')) &= \mathbf{\Delta}^{q,p}(AA''BB') \\
&= \chi_{\mathcal{A}}^{q}(AA'')\mathbf{\Gamma}^p_{\mathcal{B}(q)}(BB') \\
&= \chi_{\mathcal{A}}^{q}(A)\chi_{\mathcal{A}}^{q}(A')\mathbf{\Gamma}^p_{\mathcal{B}(q)}(B)\mathbf{\Gamma}^p_{\mathcal{B}(q)}(B') \\
&= \mathbf{\Delta}^{q,p}(AB)\mathbf{\Delta}^{q,p}(A'B').
\end{aligned}$$

The unitary property is obvious.)

(j) The set of $M(q)(= b/b(q))$ coset representatives $B_1, B_2, \ldots$ for the decomposition of $\mathcal{B}$ into right cosets with respect to $\mathcal{B}(q)$ also serve as coset representatives for the decomposition of $\mathcal{G}$ into right cosets with respect to $\mathcal{S}(q)$. (The numbers of distinct right cosets in the two decompositions are equal, as the number in the latter decomposition is $g/s(q) = (ab)/(ab(q)) = M(q)$ ($s(q)$ being the order of $\mathcal{S}(q)$). Moreover, $\mathcal{S}(q)B_j$ and $\mathcal{S}(q)B_k$ are distinct if and only if $\mathcal{B}(q)B_j$ and $\mathcal{B}(q)B_k$ are distinct. (To verify this, first suppose that $\mathcal{S}(q)B_j$ and $\mathcal{S}(q)B_k$ possess a common element. Then there exist $A, A' \in \mathcal{A}$ and $B, B' \in \mathcal{B}(q)$ such that $ABB_j = A'B'B_k$. However, as $\mathcal{S}(q)$ is a semi-direct product of $\mathcal{A}$ and $\mathcal{B}(q)$, $A = A'$ and $BB_j = B'B_k$, so that $\mathcal{B}(q)B_j$ and $\mathcal{B}(q)B_k$ possess a common element. The demonstration of the converse proposition is then obvious.)

(k) Unitary representations $\mathbf{\Gamma}^{q,p}$ of $\mathcal{G}$ of dimensions $M(q)d_p$ may be induced from the unitary representations $\mathbf{\Delta}^{q,p}$ of $\mathcal{S}(q)$ by applying the previous theorem with $\mathcal{S} = \mathcal{S}(q)$ and $\mathbf{\Delta} = \mathbf{\Delta}^{q,p}$, That is, symbolically,

$$\mathbf{\Gamma}^{q,p} = \mathbf{\Delta}^{q,p}(\mathcal{S}(q)) \uparrow \mathcal{G}.$$

Let T be any element of $\mathcal{G}$ and suppose that $T = AB$, where $A \in \mathcal{A}$ and $B \in \mathcal{B}$. By (j) the coset representatives $T_1, T_2, \ldots$ of the theorem may be identified with $B_1, B_2, \ldots$. Then $B_k(AB)B_j^{-1} = (B_kAB_k^{-1})(B_kBB_j^{-1})$, where $B_kAB_k^{-1} \in \mathcal{A}$, so $B_k(AB)B_j^{-1} \in \mathcal{S}(q)$ if and only if $B_kBB_j^{-1} \in \mathcal{B}(q)$. When $B_kBB_j^{-1} \in \mathcal{B}(q)$, Equations (5.44) and (5.46) give

$$\mathbf{\Delta}^{q,p}(B_kABB_j^{-1}) = \chi_{\mathcal{A}}^{B_k(q)}(A)\mathbf{\Gamma}^p_{\mathcal{B}(q)}(B_kBB_j^{-1}).$$

Thus, from Equations (5.41),

$$\Gamma^{q,p}(AB)_{kt,jr} = \begin{cases} \chi_{\mathcal{A}}^{B_k(q)}(A)\Gamma^p_{\mathcal{B}(q)}(B_kBB_j^{-1})_{tr}, & \text{if } B_kBB_j^{-1} \in \mathcal{B}(q), \\ 0, & \text{if } B_kBB_j^{-1} \notin \mathcal{B}(q). \end{cases} \tag{5.47}$$

Similarly, Equation (5.42) implies that the characters $\chi^{q,p}(AB)$ of $\mathbf{\Gamma}^{q,p}$ are given by

$$\chi^{q,p}(AB) = \sum_j \chi_{\mathcal{A}}^{B_j(q)}(A)\chi^p_{\mathcal{B}(q)}(B_jBB_j^{-1}), \tag{5.48}$$

where the sum is over all coset representatives B_j such that $B_jBB_j^{-1} \in \mathcal{B}(q)$, and where $\chi^p_{\mathcal{B}(q)}(B)$ are the characters of $\mathbf{\Gamma}^p_{\mathcal{B}(q)}$.

The remarkable properties of these representations $\mathbf{\Gamma}^{q,p}$ of $\mathcal{G}$ are summarized in the following theorem.

Theorem II Let $\mathbf{\Gamma}^{q,p}$ be the unitary representation of the semi-direct product group $\mathcal{G}(= \mathcal{A}\textcircled{s}\mathcal{B})$ defined by Equations (5.47). Then

(a) $\mathbf{\Gamma}^{q,p}$ is an *irreducible* representation of $\mathcal{G}$; and

(b) the *complete* set of unitary irreducible representations of $\mathcal{G}$ may be determined (up to equivalence) by choosing one q in each orbit and then constructing $\mathbf{\Gamma}^{q,p}$ for each inequivalent $\mathbf{\Gamma}^{p}_{\mathcal{B}(q)}$ of $\mathcal{B}(q)$.

Proof See, for example, Appendix C, Section 8, of Cornwell (1984).

This construction will be used in Chapter 7 in the discussion of irreducible representations of symmorphic crystallographic space groups.

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Chapter 6

Group Theory in Quantum Mechanical Calculations

1 The solution of the Schrödinger equation

One of the most valuable applications of group theory is to the solution of the Schrödinger equation. Only for a small number of very simple systems, such as the hydrogen atom, is it possible to obtain an exact analytic solution. For all other systems it is necessary to resort to numerical calculations, but the work involved can be shortened considerably by the application of group representation theory. This is particularly true in electronic energy band calculations in solid state physics, where accurate calculations are only feasible when group theoretical arguments are used to exploit the symmetry of the system to the full.

For simplicity consider the "single-particle" time-independent Schrödinger equation described in Chapter 1, Section 3(a), namely

$$H(\mathbf{r})\psi(\mathbf{r}) = \epsilon\psi(\mathbf{r}), \tag{6.1}$$

$H(\mathbf{r})$ being the Hamiltonian operator (see Equation (1.10)). It is required to find the low-lying energy eigenvalues ϵ and their corresponding eigenfunctions $\psi(\mathbf{r})$. The unknown function $\psi(\mathbf{r})$ can be expanded in terms of a complete set of known functions $\psi_1(\mathbf{r}), \psi_2(\mathbf{r}), \ldots$ that form a basis for L^2(see Appendix B, Section 3), that is,

$$\psi(\mathbf{r}) = \sum_{j=1}^{\infty} a_j \psi_j(\mathbf{r}), \tag{6.2}$$

where $a_1, a_2, \ldots$ form a set of complex numbers whose values are unknown at this stage. The assumption is now made that the series (Equation (6.2))

converges sufficiently rapidly that only the first N terms need be retained. Then it can be replaced by the approximation

$$\psi(\mathbf{r}) = \sum_{j=1}^{N} a_j \psi_j(\mathbf{r}). \tag{6.3}$$

Some judgement is required as to the best choice of the set $\psi_1(\mathbf{r}), \psi_2(\mathbf{r}), \ldots$ that will ensure the validity of this approximation. Indeed, the different types of energy band calculation, described for instance in the article of Reitz (1955), essentially differ merely in this choice. For example, in solid state problems where the valence electrons are expected to be tightly bound to the ions, it is natural to take the $\psi_j(\mathbf{r})$ to be atomic orbitals, thereby giving the so-called "method of linear combinations of atomic orbitals", often described more briefly as the "L.C.A.O. method". At the other extreme, when the valence electrons are nearly free, it is natural to form the $\psi_j(\mathbf{r})$ from plane waves (orthogonalized to the ionic electronic energy eigenfunctions to prevent the expansion giving ionic electron energy eigenfunctions), thereby giving the so-called "orthogonalized plane wave method", or "O.P.W. method" for short.

Substituting Equation (6.3) into Equation (6.1) and forming the inner product of Equation (B.18) with $\psi_k(\mathbf{r})$ gives

$$\sum_{j=1}^{N} a_j \{(\psi_k, H\psi_j) - \epsilon(\psi_k, \psi_j)\} = 0. \tag{6.4}$$

This is a matrix eigenvalue equation of the form of Equation (A.10), in which the matrix elements $(\psi_k, H\psi_j)$ are known but the eigenvalues ϵ and the elements a_j of the eigenvector are to be determined. Equation (6.4) has a non-trivial solution if and only if

$$\det\{(\psi_k, H\psi_j) - \epsilon(\psi_k, \psi_j)\} = 0, \tag{6.5}$$

in which the matrix involved is of dimension $N \times N$ (cf. Equation (A.11)). The left-hand side of the scalar equation derived from Equation (6.5) is a polynomial of degree N, the roots of which are the eigenvalues ϵ. Both the explicit determination of the polynomial and the calculation of its roots are very lengthy processes if N is large. With the roots obtained it is possible to go back to Equation (6.4), regarded now as a system of N linear algebraic equations, and for each root ϵ obtain the corresponding set of complex numbers a_j thereby giving by Equation (6.3) an approximation to the corresponding eigenfunction $\psi(\mathbf{r})$. The number N is here quite arbitrary, but clearly, as N is increased, two effects follow. Firstly, the accuracy of the approximations to the lower energy eigenvalues is improved, which is very desirable. Secondly, more eigenvalues at higher energies appear, although these are usually less important. However, as noted above, the numerical work involved increases rapidly as N increases, this work being roughly proportional to $N!$.

By invoking group representation theory this numerical work can be cut tremendously without any loss of accuracy. All that has to be done is to

arrange that the members of the complete set of known functions $\psi_j(\mathbf{r})$ of Equation (6.3) are each basis functions of the various irreducible representations of the group of the Schrödinger equation, $\mathcal{G}$. In practice this is achieved by applying the projection operators of Chapter 5, Section 1 to the atomic orbitals, orthogonalized plane waves, or other given functions that are judged appropriate to the particular system under consideration. An extra pair of indices m and p has now to be included in the designation of the functions, so that $\psi^p_{jm}(\mathbf{r})$ transforms as the mth row of the irreducible representation $\mathbf{\Gamma}^p$ of $\mathcal{G}$, the index j distinguishing linearly independent basis functions having this particular symmetry. Equation (6.3) is then rewritten as

$$\psi(\mathbf{r}) = \sum_j \sum_p \sum_{m=1}^{d_p} a^p_{jm} \psi^p_{jm}(\mathbf{r}), \tag{6.6}$$

and Equation (6.5) becomes

$$\det\{(\psi^q_{kn}, H\psi^p_{jm}) - \epsilon(\psi^q_{kn}, \psi^p_{jm})\} = 0. \tag{6.7}$$

If $\mathcal{G}$ is a finite group or a compact Lie group, each irreducible representation $\mathbf{\Gamma}^p$ may be taken to be unitary. Theorem V of Chapter 4, Section 5 then shows that

$$(\psi^q_{kn}, \psi^p_{jm}) = \delta_{qp}\delta_{nm}(\psi^p_{km}, \psi^p_{jm}). \tag{6.8}$$

Similarly, Theorem III of Chapter 5, Section 3, implies that

$$(\psi^q_{kn}, H\psi^p_{jm}) = \delta_{qp}\delta_{nm}(\psi^p_{km}, H\psi^p_{jm}). \tag{6.9}$$

The rows and columns of the determinant of Equation (6.7) may be rearranged so that all the terms corresponding to a particular row of a particular irreducible representation of $\mathcal{G}$ are grouped together. (This can be achieved by successively interchanging pairs of rows of the determinant and then pairs of columns. Such interchanges in general change the sign of a determinant. However, here the value of the determinant is zero so its value is unchanged by such a rearrangement.) Equations (6.8) and (6.9) then imply that the determinant of Equation (6.7) takes the "block form"

$$\det \begin{bmatrix} \mathbf{D}(1,1) & \mathbf{0} & \dots & \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots \\ \mathbf{0} & \mathbf{D}(1,2) & \dots & \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \\ \mathbf{0} & \mathbf{0} & \dots & \mathbf{D}(1,d_1) & \mathbf{0} & \mathbf{0} & \dots \\ \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} & \mathbf{D}(2,1) & \mathbf{0} & \dots \\ \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} & \mathbf{0} & \mathbf{D}(2,2) & \dots \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \end{bmatrix} = 0, \tag{6.10}$$

where $\mathbf{D}(p,m)$ is a submatrix defined by

$$D(p,m)_{kj} = (\psi^p_{km}, H\psi^p_{jm}) - \epsilon(\psi^p_{km}, \psi^p_{jm}).$$

Thus $\mathbf{D}(p,m)$ involves *only* basis functions corresponding to the mth row of $\mathbf{\Gamma}^p$. The matrices $\mathbf{0}$ consist entirely of zero elements. Equation (6.10) can be factorized to give

$$\prod_p \prod_{m=1}^{d_p} \det \mathbf{D}(p,m) = 0.$$

The complete set of eigenvalues of Equation (6.10) are then obtained by taking

$$\det \mathbf{D}(p,m) = 0 \tag{6.11}$$

for every p and every $m = 1, 2, \ldots, d_p$. *The energy eigenvalues corresponding to the mth row of* $\mathbf{\Gamma}^p$ *are therefore given by the secular equation, Equation (6.11), which only involves basis functions corresponding to the mth row of* $\mathbf{\Gamma}^p$. As the dimensions of $\mathbf{D}(p,m)$ are usually very much smaller than those of the determinant of Equation (6.7), very much less numerical work is now needed to find the energy eigenvalues and eigenfunctions for the same degree of accuracy.

A further valuable saving of effort is provided by noting that Equations (6.8) and (6.9) also imply that

$$\mathbf{D}(p,1) = \mathbf{D}(p,2) = \ldots = \mathbf{D}(p,d_p) \tag{6.12}$$

for each irreducible representation $\mathbf{\Gamma}^p$. Thus *only one* secular equation (Equation (6.11)) has to be solved for each irreducible representation $\mathbf{\Gamma}^p$ and each of the resulting energy eigenvalues can be taken to be d_p-fold degenerate.

It is very interesting to relate these results to the general conclusion drawn in Chapter 1, Section 4, that every d-fold degenerate energy eigenvalue is associated with a d-dimensional representation $\mathbf{\Gamma}$ of the group of the Schrödinger equation, the corresponding d linearly independent eigenfunctions being basis functions of this representation .

Suppose first that this representation $\mathbf{\Gamma}$ is irreducible and is identical to $\mathbf{\Gamma}^p$. Then the d-fold degeneracy of the energy eigenvalue follows automatically from the identities in Equations (6.12). It is not unexpected that the energy eigenfunction $\psi(\mathbf{r})$ transforming as the mth row of $\mathbf{\Gamma}^p$ involves only basis functions transforming the same way. That is, $a_{kn}^q = O$ for $q \neq p$ and $n \neq m$ in the expansion in Equation (6.6).

The situation when $\mathbf{\Gamma}$ is reducible is more complicated. Suppose that $\mathbf{\Gamma}$ is the direct sum of two inequivalent irreducible representations $\mathbf{\Gamma}^p$ and $\mathbf{\Gamma}^q$ of dimensions d_p and d_q, so that $d = d_p + d_q$. Then d_p of the energy eigenfunctions can be taken as basis functions of $\mathbf{\Gamma}^p$, the remaining d_q eigenfunctions being basis functions of $\mathbf{\Gamma}^q$. The identities in Equations (6.12) produce a d_p-fold degeneracy in the energy eigenvalue. Similarly, the corresponding identities with p replaced by q give rise to a d_q-fold degeneracy. The overall $d(= d_p + d_q)$-fold degeneracy must be a consequence of the secular equations $\det \mathbf{D}(p,m) = 0$ and $\det \mathbf{D}(q,n) = 0$ possessing a common eigenvalue, but no reason for this can be attributed to the symmetry of the system. Consequently the extra degeneracy associated with this common eigenvalue is called an "accidental"

degeneracy, and the energy levels corresponding to $\mathbf{\Gamma}^p$ and $\mathbf{\Gamma}^q$ are said to "stick together". In general, an arbitrarily small change in the potential that preserves its symmetry will break the accidental degeneracy.

It is to be expected that accidental degeneracies occur only very rarely, the normal situation being that in which the representation $\mathbf{\Gamma}$ is irreducible. However, in some exceptional systems, such as the hydrogen atom, these accidental degeneracies occur so extensively and in such a regular fashion that they cannot be truly coincidental. Their origin lies in a "hidden" symmetry which gives rise to an invariance group that is larger than the obvious invariance group. For the hydrogen atom the situation is described in detail in, for example, Chapter 12, Section 8, of Cornwell (1984).

2 Transition probabilities and selection rules

Suppose that a small time-dependent perturbation $H'(t)$ is applied to a system whose time-independent "unperturbed" Hamiltonian is H_0, so that the total Hamiltonian becomes

$$H(t) = H_0 + H'(t).$$

Suppose that before the perturbation is applied (that is, at time $t = -\infty$) the system is in an eigenstate ϕ_i of H_0 with energy eigenvalue ϵ_i. Then, according to first-order perturbation theory (Schiff 1968), the probability of finding the system at time t in another eigenstate ϕ_f of H_0 (whose energy eigenvalue is ϵ_f) is given by

$$|(i\hbar)^{-1} \int_{-\infty}^{\infty} (\phi_f, H'(t')\phi_i) \exp\{i(\epsilon_f - \epsilon_i)t'/\hbar\}\, dt'|^2.$$

(Here it is assumed that ϕ_i and ϕ_f have been appropriately normalized.)

The significant part of this expression is the inner product $(\phi_f, H'(t')\phi_i)$. The analysis of Chapter 1, Section 4 shows that ϕ_i and ϕ_f must be basis functions of some representations of the invariance group $\mathcal{G}_0$ of the unperturbed Hamiltonian H_0. With the perturbation $H'(t')$ expressed in terms of irreducible tensor operators of $\mathcal{G}_0$, such inner products can be studied using the Wigner-Eckart Theorem of Chapter 5, Section 3. In particular, it is possible to deduce when symmetry requires that $(\phi_f, H'(t')\phi_i) = 0$. When this is so, transitions from ϕ_i to ϕ_f are *forbidden* (at least in first-order perturbation theory).

This basic idea will now be developed for the very important case in which the system interacts with an external electromagnetic field, resulting in absorption or induced emission of radiation. It will be assumed that the unperturbed system is described by a "single-particle" Schrödinger equation (in the sense of Chapter 1, Section 3(a)), so that (cf. Equation (1.10))

$$H_0(\mathbf{r}) = \frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(\mathbf{r}),$$

where μ is the mass of the particle and $V(\mathbf{r})$ the potential that it experiences. The perturbing operator $H'(\mathbf{r}, t)$ may be taken to be

$$H'(\mathbf{r}, t) = (ie\hbar/\mu c)\mathbf{A}(\mathbf{r}, t).\mathbf{grad}, \tag{6.13}$$

where c is the speed of light and the vector potential $\mathbf{A}(\mathbf{r}, t)$ for a plane electromagnetic wave with wave vector $\mathbf{k}$ and frequency $\omega/2\pi$ is of the form

$$\mathbf{A}(\mathbf{r}, t) = 2\mathbf{A}_0 \cos(\mathbf{k}.\mathbf{r} - \omega t + \alpha).$$

Here $\mathbf{A}_0$ is a constant vector, with real components, that specifies the polarization of the radiation, α gives its phase, $\mathbf{A}_0.\mathbf{k} = 0$, and $\omega = |\mathbf{k}|c$. Then the transition probability for *absorption* of a photon from the radiation field causing a transition from $\phi_i(\mathbf{r})$ to $\phi_f(\mathbf{r})$ is given by

$$\frac{4\pi^2 e^2 \hbar^2 I((\epsilon_f - \epsilon_i)/\hbar)}{\mu^2 c^2 (\epsilon_f - \epsilon_i)^2} |(\phi_f, \mathbf{A}_0.\mathbf{grad}\phi_i)|^2, \tag{6.14}$$

the angular frequency of the absorbed radiation being $(\epsilon_f - \epsilon_i)/\hbar$. Similarly, the transition probability for *induced emission* of a photon associated with a transition from $\phi_i(\mathbf{r})$ to $\phi_f(\mathbf{r})$ is given by

$$\frac{4\pi^2 e^2 \hbar^2 I((\epsilon_i - \epsilon_f)/\hbar)}{\mu^2 c^2 (\epsilon_i - \epsilon_f)^2} |(\phi_f, \mathbf{A}_0.\mathbf{grad}\phi_i)|^2, \tag{6.15}$$

the angular frequency of the emitted radiation being $(\epsilon_i - \epsilon_f)/\hbar$. In Expressions (6.14) and (6.15) $I(\omega)$ is defined to be such that the intensity of the radiation field in the angular frequency range ω to $\omega + d\omega$ is $I(\omega)d\omega$. In deriving Expressions (6.14) and (6.15) it has been assumed that the wavelength of the radiation is much greater than the dimensions of the regions in which the eigenfunctions $\phi_i(\mathbf{r})$ and $\phi_f(\mathbf{r})$ are significantly different from zero. As the inner products of Expressions (6.14) and (6.15) can be rewritten in the form

$$(\phi_f, \mathbf{A}_0.\mathbf{grad}\phi_i) = -\{\mu(\epsilon_f - \epsilon_i)/\hbar^2\}(\phi_f, \mathbf{A}_0.\mathbf{r}\phi_i), \tag{6.16}$$

the transitions are often called "electric dipole transitions". (The detailed derivations of Expressions (6.13), (6.14), (6.15) and (6.16) may be found in the book by Schiff (1968).)

It is interesting to note (see Schiff (1968)) that the transition probability for *spontaneous* emission of radiation of frequency $(\epsilon_i - \epsilon_f)/\hbar$ polarized in the direction of the unit vector $\mathbf{n}$ in a transition from $\phi_i(\mathbf{r})$ to $\phi_f(\mathbf{r})$ is given by

$$\frac{4e^2(\epsilon_i - \epsilon_f)}{3c^2\mu^2} |(\phi_f, \mathbf{n}.\mathbf{grad}\phi_i)|^2.$$

Equation (6.16) allows this too to be expressed in terms of "dipole" inner products.

Let $Q = \mathbf{A}_0.\mathbf{grad}$ for absorption or induced emission and $Q = \mathbf{n}.\mathbf{grad}$ for spontaneous emission. Then Example III of Chapter 5, Section 3 shows that

Q is easily expressed as a linear combination of irreducible tensor operators. There is no intrinsic difficulty in carrying out the analysis for the most general case, but for simplicity it will be assumed that Q is an irreducible tensor operator transforming as the kth row of the unitary irreducible representation $\mathbf{\Gamma}_0^q$ of $\mathcal{G}_0$. Suppose also that $\phi_i(\mathbf{r}) = \phi_j^p(\mathbf{r})$ and $\phi_f(\mathbf{r}) = \phi_l^r(\mathbf{r})$, where $\phi_j^p(\mathbf{r})$ and $\phi_l^r(\mathbf{r})$ are respectively basis functions transforming as the jth and lth rows of the unitary irreducible representations $\mathbf{\Gamma}_0^p$ and $\mathbf{\Gamma}_0^r$ of $\mathcal{G}_0$. If $\mathcal{G}_0$ is a finite group or a compact Lie group, the Wigner-Eckart Theorem shows that

$$(\phi_f, Q\phi_i) = 0$$

if $n_{pq}^r = 0$, that is, if $\mathbf{\Gamma}_0^r$ does *not* appear in the reduction of $\mathbf{\Gamma}_0^p \otimes \mathbf{\Gamma}_0^q$. Thus a list of forbidden transitions can be found from the Clebsch-Gordan *series* alone. However, a *complete* list requires a knowledge of the Clebsch-Gordan coefficients, for if $n_{pq}^r \neq 0$ the Wigner-Eckart Theorem implies that

$$(\phi_f, Q\phi_i) = \sum_{\alpha=1}^{n_{pq}^r} \left(\begin{array}{cc|cc} p & q & r, & \alpha \\ j & k & l & \end{array} \right)^\star (r|Q|p)_\alpha, \tag{6.17}$$

and it can happen that

$$\left(\begin{array}{cc|cc} p & q & r, & \alpha \\ j & k & l & \end{array} \right) = 0$$

for all $\alpha = 1, 2, \ldots, n_{pq}^r$, thereby giving again a zero transition probability. (This situation occurs in the example that will be given shortly.)

The Wigner-Eckart Theorem can also be employed in the analysis of the magnitudes of the transition probabilities of the allowed transitions. If $n_{pq}^r \neq 0$, Equation (6.17) shows that $(\phi_f, Q\phi_i)$ depends on n_{pq}^r reduced matrix elements. The transition probabilities for all other transitions involving initial states that are partners of $\phi_i(\mathbf{r})$ in the same basis, final states that are partners of $\phi_f(\mathbf{r})$ in the same basis, and other directions of polarization whose operators form part of the same set of irreducible tensor operators as Q also depend on the Clebsch-Gordan coefficients and these n_{pq}^r reduced matrix elements. Thus a complete description of $d_p d_q d_r$ possible transitions depends only on n_{pq}^r reduced matrix elements, where n_{pq}^r can be considerably smaller than $d_p d_q d_r$.

The most important case is that in which $\mathcal{G}_0$ is the group of all rotations in $\mathbb{R}^3$. This will be considered in detail in Chapter 10, Section 6, after the irreducible representations of this group have been derived. The following simple example will serve until then to illustrate the power of the technique.

Example I *Optical selection rules associated with the crystallographic point group* D_4

Let $\mathcal{G}_0 = D_4$ and let $\mathbf{\Gamma}_0^p$ denote the irreducible representations of D_4 previously referred to as $\mathbf{\Gamma}^p$, $p = 1, 2, 3, 4, 5$. Consider absorption from an initial state

$\phi_i(\mathbf{r})$ that transforms as the first row of the two-dimensional irreducible representation $\Gamma_0^5 (= \Gamma^5)$ (the explicit matrices being as in Example I of Chapter 5, Section 1).

For polarization vector $\mathbf{A}_0$ in the x-direction, $\mathbf{A}_0.\mathbf{grad} = A_{01}\partial/\partial x$, which (by Example III of Chapter 5, Section 3) is an irreducible tensor operator transforming as the first row of Γ_0^5. As $\Gamma_0^5 \otimes \Gamma_0^5 = \Gamma_0^1 \oplus \Gamma_0^2 \oplus \Gamma_0^3 \oplus \Gamma_0^4$ (see Example I of Chapter 5, Section 2), the Clebsch-Gordan series implies that the final state $\phi_f(\mathbf{r})$ cannot transform as either row of Γ_0^5. However, the Clebsch-Gordan coefficients (see Example I of Chapter 5, Section 3) show that $\phi_f(\mathbf{r})$ can only transform as Γ_0^1 or Γ_0^2.

Similarly, for $\mathbf{A}_0$ in the y-direction, $\mathbf{A}_0.\mathbf{grad} = A_{02}\partial/\partial y$, which is an irreducible tensor operator transforming as Γ_0^3. As $\Gamma_0^5 \otimes \Gamma_0^3 \approx \Gamma_0^5$ transitions can only occur to final states $\phi_f(\mathbf{r})$ transforming as Γ_0^5. Examination of the Clebsch-Gordan coefficients shows that $\phi_f(\mathbf{r})$ must transform as the second row of Γ_0^5.

Finally, for $\mathbf{A}_0$ in the z-direction, $\mathbf{A}_0.\mathbf{grad} = A_{03}\partial/\partial z$, an irreducible tensor operator transforming as the second row of Γ_0^5. Again the Clebsch-Gordan series indicates that $\phi_f(\mathbf{r})$ cannot transform as either row of Γ_0^5, while the Clebsch-Gordan coefficients show that $\phi_f(\mathbf{r})$ can only transform as Γ_0^3 or Γ_0^4.

3 Time-independent perturbation theory

Suppose that the Hamiltonian H of a system is time-independent and is made up of two time-independent parts H_0 and H', where H_0 is sufficiently simple that its eigenfunctions and eigenvalues are known, and H' is sufficiently small that its effect can be considered to be a perturbation on H_0. The problem is then to find the eigenfunctions and eigenvalues of $H = H_0 + H'$ in terms of those of H_0. It is assumed that the eigenfunctions of H and H_0 can be put into a one-to-one correspondence, in the sense that they are the limits as $\lambda \to 0$ and $\lambda \to 1$ respectively of the eigenfunctions of the operator $H_0 + \lambda H'$, $0 \leq \lambda \leq 1$. If $\phi_1, \phi_2, \ldots, \phi_d$ are a set of eigenfunctions of H_0 corresponding to the d-fold degenerate energy eigenvalue ϵ_0 and the associated eigenfunctions $\psi_1, \psi_2, \ldots, \psi_d$ of H correspond to eigenvalues that are not equal to each other, then the perturbation H' may be said to "split" ϵ_0.

It will be shown that a considerable amount of information about such splittings can be found very simply using group representation theory. For simplicity it will be assumed that H and H_0 give "single- particle" Schrödinger equations (in the sense of Chapter 1, Section 3(a)). Let $\mathcal{G}_0$ and $\mathcal{G}$ be the invariance groups of H_0 and H respectively. Usually there exists a coordinate transformation T of H_0 such that

$$H'(\{\mathbf{R}(T)|\mathbf{t}(T)\}\mathbf{r}) \neq H'(\mathbf{r}),$$

so that Equation (1.13) implies that $\mathcal{G}$ is a proper subgroup of $\mathcal{G}_0$. Suppose that the unperturbed energy eigenvalue ϵ_0 corresponds to a representation Γ_0

of $\mathcal{G}_0$. Then $\mathbf{\Gamma}_0$ provides a representation of the subgroup $\mathcal{G}$. However, even if $\mathbf{\Gamma}_0$ is an irreducible representation of $\mathcal{G}_0$, as a representation of $\mathcal{G}$ $\mathbf{\Gamma}_0$ may be reducible. For convenience it will be assumed that $\mathcal{G}$ is a finite group or a compact Lie group, so that $\mathbf{\Gamma}_0$ is then completely reducible on $\mathcal{G}$ (see Chapter 4, Section 4). Thus suppose that as a representation of $\mathcal{G}$

$$\mathbf{\Gamma}_0 \approx \sum_r \oplus n_r \mathbf{\Gamma}^r, \tag{6.18}$$

where the sum is over all inequivalent unitary irreducible representations $\mathbf{\Gamma}^r$ of $\mathcal{G}$, n_r being the number of times that $\mathbf{\Gamma}^r$ appears in the reduction of $\mathbf{\Gamma}_0$. Here n_r may be zero for some $\mathbf{\Gamma}^r$. These integers are easily evaluated from a knowledge of the characters of $\mathcal{G}_0$ and $\mathcal{G}$ alone, for Theorem V of Chapter 4, Section 6 gives

$$n_r = (1/g) \sum_{T \in \mathcal{G}} \chi_0(T) \chi^r(T)^\star$$

for the case in which $\mathcal{G}$ is finite and of order g. Here $\chi_0(T)$ and $\chi^p(T)$ denote the characters of $\mathbf{\Gamma}_0$ and $\mathbf{\Gamma}^r$ respectively. Similarly, if $\mathcal{G}$ is a compact Lie group,

$$n_r = \int_{\mathcal{G}} \chi_0(T) \chi^r(T)^\star \, dT.$$

Suppose that $\sum_r n_r = n$, so that Equation (6.18) contains n irreducible representations of $\mathcal{G}$. Then the d perturbed energy eigenfunctions ψ_1, ψ_2, ...,ψ_d in general belong to n different eigenvalues of H. Thus ϵ_0 is split by the perturbation H' into n different values. If d_r is the dimension of $\mathbf{\Gamma}^r$, then the perturbed energy eigenvalue corresponding to $\mathbf{\Gamma}^r$ is d_r-fold degenerate. Naturally $\sum_r d_r = d$. As $d_r = \chi^r(E)$, both the number of perturbed energy eigenvalues and their degeneracies can be predicted using the *characters* of $\mathcal{G}_0$ and $\mathcal{G}$ alone.

In the special case in which $\mathbf{\Gamma}_0$ provides an *irreducible* representation of $\mathcal{G}$, the unperturbed eigenvalue ϵ_0 is not split. (In particular, this happens when $\mathcal{G}$ coincides with $\mathcal{G}_0$ and $\mathbf{\Gamma}_0$ is an irreducible representation of $\mathcal{G}_0$.)

As all expressions for the perturbed eigenvalues and eigenfunctions involve only the unperturbed energy eigenvalues and matrix elements of H' between unperturbed energy eigenvalues (Schiff 1968), the Wigner-Eckart Theorem of Chapter 5, Section 3, can be brought into use again. For example, suppose that $\mathbf{\Gamma}_0$ is equal to $\mathbf{\Gamma}_0^p$, a unitary irreducible representation of $\mathcal{G}_0$, and $\phi_1^p(\mathbf{r}), \phi_2^p(\mathbf{r}), \ldots, \phi_d^p(\mathbf{r})$ are a set of linearly independent eigenfunctions of H_0, with eigenvalue ϵ_0, that are basis functions for $\mathbf{\Gamma}_0^p$. Suppose also that H' is an irreducible tensor operator transforming as the kth row of a unitary irreducible representation $\mathbf{\Gamma}_0^q$ of $\mathcal{G}_0$. Then, if $d = 1$ (that is, if ϵ_0 is "non-degenerate"), the corresponding perturbed eigenvalue ϵ is given to first order by

$$\epsilon = \epsilon_0 + (\phi_1^p, H' \phi_1^p),$$

while if $d > 1$ the corresponding first-order perturbed eigenvalues are the eigenvalues of the $d \times d$ matrix $\mathbf{A}$ whose elements are given by

$$A_{lj} = \epsilon_0 \delta_{lj} + (\phi_l^p, H' \phi_j^p), \tag{6.19}$$

$j, l = 1, 2, \ldots, d$. In both cases there is a first-order effect only if $\mathbf{\Gamma}_0^p \otimes \mathbf{\Gamma}_0^q$ contains $\mathbf{\Gamma}_0^p$ (that is, when $n_{pq}^p \neq 0$). When this is so the Wigner-Eckart Theorem shows that

$$(\phi_l^p, H' \phi_j^p) = \sum_{\alpha=1}^{n_{pq}^r} \left(\begin{array}{cc|cc} p & q & p, & \alpha \\ j & k & l & \end{array} \right)^\star (p|H'|p)_\alpha, \tag{6.20}$$

so that the matrix elements depend on the Clebsch-Gordan coefficients and n_{pq}^p reduced matrix elements.

For a further analysis of the case $d > 1$, see, for example, Chapter 6, Section 3, of Cornwell (1984).

Chapter 7

Crystallographic Space Groups

1 The Bravais lattices

An infinite three-dimensional lattice may be defined in terms of three linearly independent real "basic lattice vectors" $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$. The set of all lattice vectors of the lattice is then given by

$$\mathbf{t}_\mathbf{n} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3,$$

where $\mathbf{n} = (n_1, n_2, n_3)$, and n_1, n_2 and n_3 are integers that take all possible values, positive, negative and zero. Points in $\mathbb{R}^3$ having lattice vectors as their position vectors are called "lattice points" and a pure translation through a lattice vector $\mathbf{t}_\mathbf{n}$, $\{\mathbf{1}|\mathbf{t}_\mathbf{n}\}$, is called a "primitive" translation.

Suppose that in a crystalline solid there are S nuclei per lattice point, and that the equilibrium positions of the nuclei associated with the lattice point $\mathbf{r} = \mathbf{0}$ have position vectors $\boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \ldots, \boldsymbol{\tau}_S$. Then the equilibrium positions of the whole set of nuclei are given by

$$\mathbf{r}^e_{\mathbf{n}\gamma} = \mathbf{t}_\mathbf{n} + \boldsymbol{\tau}_\gamma, \tag{7.1}$$

where $\gamma = 1, 2, \ldots, S$ and $\mathbf{t}_\mathbf{n}$ is any lattice vector. In the special case when $S = 1$, $\boldsymbol{\tau}_1$ may be taken to be $\mathbf{0}$ and the index γ may be omitted, so that $\mathbf{r}^e_\mathbf{n} = \mathbf{t}_\mathbf{n}$.

The set of all primitive translations of a lattice form a group which will be denoted by $\mathcal{T}^\infty$. $\mathcal{T}^\infty$ is Abelian but of infinite order. In Section 2 the Born cyclic boundary conditions will be introduced. They have the effect of replacing this infinite group by a similar group of large but finite order, so that all the theorems on finite groups of the previous chapters apply.

The "maximal point group" $\mathcal{G}_0^{max}$ of a crystal lattice may be defined as the set of all pure rotations $\{\mathbf{R}(T)|\mathbf{0}\}$ such that, for every lattice vector $\mathbf{t}_\mathbf{n}$,

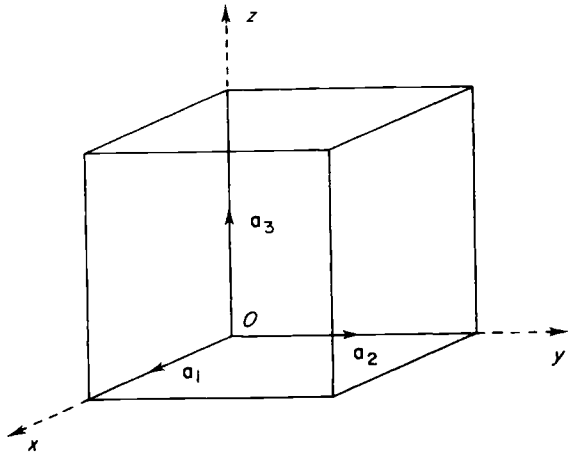

Figure 7.1: Basic lattice vectors of the simple cubic lattice, Γ_c.

the quantity $\mathbf{R}(T)\mathbf{t_n}$ is also a lattice vector. Clearly $\mathbf{R}(T) \in \mathcal{G}_0^{max}$ if and only if $\mathbf{R}(T)\mathbf{a}_j$ is a lattice vector for $j = 1, 2, 3$.

There are essentially 14 different types of crystal lattice. They are known as the "Bravais lattices". These will be described briefly, but no attempt will be made to give a logical derivation or to show that there are no others. (In this context two types of lattice are regarded as being different if they have different maximal point groups, even though one type is a special case of the other. For example, as may be seen from Table 7.1, the simple cubic lattice Γ_c is a special case of the simple tetragonal lattice Γ_q with $a = b$, but $\mathcal{G}_0^{max} = O_h$ for Γ_c, whereas $\mathcal{G}_0^{max} = D_{4h}$ for Γ_q.)

Lattices with the same maximal point group are said to belong to the same "symmetry system", there being only seven different symmetry systems. Complete details are given in Table 7.1, in which the notation for point groups is that of Schönfliess (1923). (A full specification of these and the other crystallographic point groups may be found in Appendix C.)

The cubic system is probably the most significant, the body-centred and face-centred lattices occurring for a large number of important solids. The basic lattice vectors of the cubic lattices are shown in Figures 7.1, 7.2 and 7.3. The lattice points of the simple cubic lattice Γ_c merely form a repeated cubic array, and the basic lattice vectors lie along three edges of a cube. For the body-centred cubic lattice Γ_c^v the basic lattice vectors join a point at the centre of a cube to three of the vertices of the cube, so that the lattice points form a repeated cubic array with lattice points also occurring at every cube centre. For the face-centred lattice Γ_c^f the lattice points again form a repeated cubic array with additional points also occurring at the midpoints of every cube face, the basic lattice vectors then joining a cube vertex to the midpoints of the three adjacent cube faces.

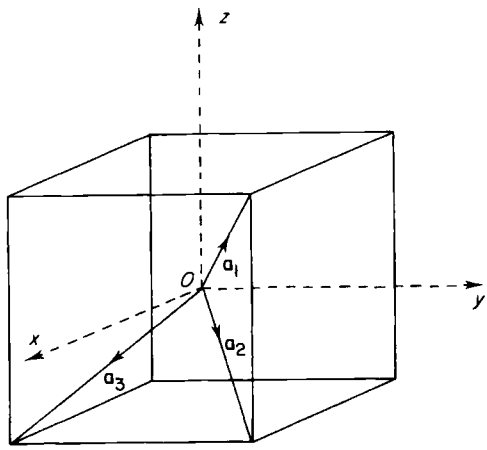

Figure 7.2: Basic lattice vectors of the body-centred cubic lattice, Γ_c^v.

A symmetry system α may be regarded as being "subordinate" to a symmetry system β if $\mathcal{G}_0^{max}$ for α is a subgroup of $\mathcal{G}_0^{max}$ for β and at least one lattice of β is a special case of a lattice of α. The complete subordination scheme is then:

triclinic $<$ monoclinic $<$ orthorhombic $<$ tetragonal $<$ cubic;

monoclinic $<$ rhombohedral; orthorhombic $<$ hexagonal;

(Here $\alpha < \beta$ indicates that α is subordinate to β.)

For a perfect crystalline solid the group of the Schrödinger equation is a crystallographic space group, which contains rotations as well as pure primitive translations. The crystallographic space groups will be investigated in detail in Section 6. However, it is very enlightening, as a first stage in their study, to limit attention to the subgroup $\mathcal{T}$ of pure primitive translations of the relevant lattice. Only the translational symmetry is then being taken into account.

In particular, the energy eigenfunctions must transform according to the irreducible representations of this subgroup, which is equivalent to saying that they satisfy Bloch's Theorem, as will be demonstrated in Section 3. Bloch's Theorem has now become so much an essential part of the theory of solids that it is sometimes forgotten that it is basically a group theoretical result. The elementary energy band theory based upon Bloch's Theorem itself requires no knowledge of group theory and so is presented in most textbooks on solid state theory. However, the neglect of rotational symmetries in this elementary theory does mean that some phenomena are overlooked, and, in particular, it cannot predict the extra degeneracies which can occur in electronic energy levels. Moreover, it is only by taking into account the rotational symmetries that it is possible to reduce the numerical work in energy band calculations to a manageable amount and still produce accurate results.

(1) Triclinic symmetry system ($\mathcal{G}_0^{max} = C_i$):
  (i) simple triclinic lattice, Γ_t: $\mathbf{a}_1, \mathbf{a}_2$ and $\mathbf{a}_3$ arbitrary.

(2) Monoclinic symmetry system ($\mathcal{G}_0^{max} = C_{2h}$):
  (i) simple monoclinic lattice, Γ_m:
    $\mathbf{a}_3$ perpendicular to both $\mathbf{a}_1$ and $\mathbf{a}_2$;
  (ii) base-centred monoclinic lattice, Γ_m^b:
    $\mathbf{a}_1 = (a, b, 0)$, $\mathbf{a}_2 = (a, -b, 0)$, $\mathbf{a}_3 = (c, 0, d)$.

(3) Orthorhombic symmetry system ($\mathcal{G}_0^{max} = D_{2h}$):
  (i) simple orthorhombic lattice, Γ_o:
    $\mathbf{a}_1 = (a, 0, 0)$, $\mathbf{a}_2 = (0, b, 0)$, $\mathbf{a}_3 = (0, 0, c)$;
  (ii) base-centred orthorhombic lattice, Γ_o^b:
    $\mathbf{a}_1 = (a, b, 0)$, $\mathbf{a}_2 = (a, -b, 0)$, $\mathbf{a}_3 = (0, 0, c)$;
  (iii) body-centred orthorhombic lattice, Γ_o^v:
    $\mathbf{a}_1 = (a, b, c)$, $\mathbf{a}_2 = (a, b, -c)$, $\mathbf{a}_3 = (a, -b, -c)$;
  (iv) face-centred orthorhombic lattice, Γ_o^f:
    $\mathbf{a}_1 = (a, b, 0)$, $\mathbf{a}_2 = (0, b, c)$, $\mathbf{a}_3 = (a, 0, c)$.

(4) Tetragonal symmetry system ($\mathcal{G}_0^{max} = D_{4h}$):
  (i) simple tetragonal lattice, Γ_q:
    $\mathbf{a}_1 = (a, 0, 0)$, $\mathbf{a}_2 = (0, a, 0)$, $\mathbf{a}_3 = (0, 0, b)$;
  (ii) body-centred tetragonal lattice, Γ_q^v:
    $\mathbf{a}_1 = (a, a, b)$, $\mathbf{a}_2 = (a, a, -b)$, $\mathbf{a}_3 = (a, -a, b)$.

(5) Cubic symmetry system ($\mathcal{G}_0^{max} = O_h$):
  (i) simple cubic lattice, Γ_c:
    $\mathbf{a}_1 = (a, 0, 0)$, $\mathbf{a}_2 = (0, a, 0)$, $\mathbf{a}_3 = (0, 0, a)$;
  (ii) body-centred cubic lattice, Γ_c^v:
    $\mathbf{a}_1 = \frac{1}{2}a(1, 1, 1)$, $\mathbf{a}_2 = \frac{1}{2}a(1, 1, -1)$, $\mathbf{a}_3 = \frac{1}{2}a(1, -1, -1)$;
  (iii) face-centred cubic lattice, Γ_c^f:
    $\mathbf{a}_1 = \frac{1}{2}a(1, 1, 0)$, $\mathbf{a}_2 = \frac{1}{2}a(0, 1, 1)$, $\mathbf{a}_3 = \frac{1}{2}a(1, 0, 1)$.

(6) Rhombohedral (or trigonal) symmetry system ($\mathcal{G}_0^{max} = D_{3d}$):
  (i) simple rhombohedral lattice, Γ_{rh}:
    $\mathbf{a}_1 = (a, 0, b)$, $\mathbf{a}_2 = (\frac{1}{2}a\sqrt{3}, -\frac{1}{2}a, b)$, $\mathbf{a}_3 = (-\frac{1}{2}a\sqrt{3}, -\frac{1}{2}a, b)$.

(7) Hexagonal symmetry system ($\mathcal{G}_0^{max} = D_{6h}$):
  (i) simple hexagonal lattice, Γ_h:
    $\mathbf{a}_1 = (0, 0, c)$, $\mathbf{a}_2 = (a, 0, 0)$, $\mathbf{a}_3 = (-\frac{1}{2}a, -\frac{1}{2}a\sqrt{3}, 0)$.

Table 7.1: The Bravais lattices. (The real parameters a, b, c and d are arbitrary.)

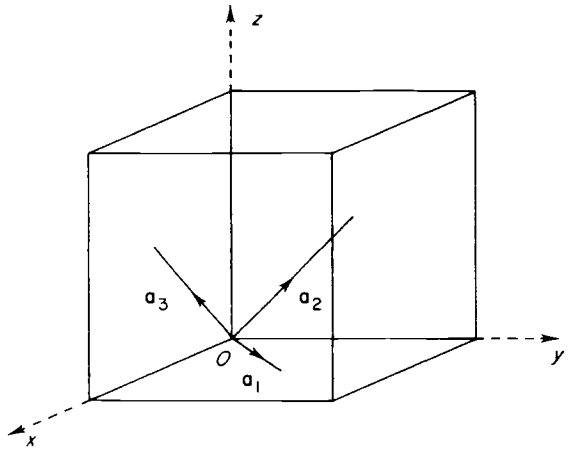

Figure 7.3: Basic lattice vectors of the face-centred cubic lattice, Γ_c^f.

A proof of Bloch's Theorem that involves only an elementary application of the ideas of the previous chapters is given is Section 3. Sections 4 and 5 are then devoted to a brief account of the elementary electronic energy band theory that is based on this theorem. Section 8 then describes, for the case of symmorphic space groups, how this theory is modified when the full space group is introduced in place of its translational subgroup $\mathcal{T}$. It will be seen there that the concepts introduced in Sections 4 and 5 still play a fundamental role.

2 The cyclic boundary conditions

Strictly speaking, a real crystalline solid cannot possess any translational symmetry because it is necessarily finite in extent. Consequently any translation will shift some electron or nucleus from just inside some surface to the outside of the body, that is, to a completely different environment.

On the other hand, for a normal sample the inter-nuclear spacing is so much smaller than the dimensions of the sample and the interactions that directly affect each electron or nucleus are of such short range, that for electrons and nuclei well inside the body the situation is almost exactly as if the solid were infinite in extent. Moreover, the evidence of X-ray crystallography is that the nuclei within a solid can be ordered as if they were based on an infinite lattice, except near the surfaces. As most of the properties of a solid depend only on the behaviour of the vast majority of electrons or nuclei that lie in the interior, it is a very reasonable approximation to idealize the situation by working with models based on infinite lattices. The translational symmetry possessed by such models then permits a considerable simplification of the analysis.

However, the symmetry groups based on infinite lattices are necessarily of infinite order, and it is easier to work with groups of finite order. This can be achieved by imposing "cyclic" boundary conditions on the infinite lattice.

For the electrons it may be assumed that for every energy eigenfunction $\phi(\mathbf{r})$

$$\phi(\mathbf{r}) = \phi(\mathbf{r} + N_1\mathbf{a}_1) = \phi(\mathbf{r} + N_2\mathbf{a}_2) = \phi(\mathbf{r} + N_3\mathbf{a}_3), \tag{7.2}$$

where N_1, N_2 and N_3 are very large positive integers and $\mathbf{a}_1, \mathbf{a}_2$ and $\mathbf{a}_3$ are the basic lattice vectors of the lattice. This implies that the infinite crystal is considered to consist of a set of basic blocks in the form of parallelepipeds having edges $N_1\mathbf{a}_1$, $N_2\mathbf{a}_2$ and $N_3\mathbf{a}_3$, and that the physical situation is identical in corresponding points of different blocks. These boundary conditions cannot affect the behaviour of electrons well inside each basic block to any significant extent, so the bulk properties are again unchanged. The integers N_1, N_2 and N_3 may be taken to be as large as desired.

The integration involved in the inner product (ϕ, ψ) defined in Equation (1.19) must now be taken as being over just one basic block of the crystal, B. For any pure primitive translation T the operators $P(T)$ retain the unitary property of Equation (1.20), provided all functions involved satisfy Equation (7.2). This follows because $(P(T)\phi, P(T)\psi)$ is equal to

$$\int\int\int_B \phi(\mathbf{r} - \mathbf{t}(T))^* \psi(\mathbf{r} - \mathbf{t}(T))\, dxdydz = \int\int\int_{B'} \phi(\mathbf{r})^* \psi(\mathbf{r})\, dxdydz,$$

where B' is obtained from B by a translation $-\mathbf{t}(T)$. As every part of B' can be mapped into a part of B by an appropriate combination of translations through $N_1\mathbf{a}_1$, $N_2\mathbf{a}_2$ and $N_3\mathbf{a}_3$, by Equations (7.2) the last integral becomes (ϕ, ψ).

The conditions in Equations (7.2) are often referred to as the "Born cyclic boundary conditions", as they are the analogues for electronic states of the vibrational boundary conditions first proposed by Born and von Karman (1912). They imply that

$$P(\{\mathbf{1}|N_j\mathbf{a}_j\}) = P(\{\mathbf{1}|\mathbf{0}\}) \tag{7.3}$$

for every function of interest and for $j = 1, 2, 3$. (Of course $P(\{\mathbf{1}|\mathbf{0}\})$ is merely the identity operator.) Consequently

$$P(\{\mathbf{1}|\mathbf{t}_\mathbf{n} + l_1N_1\mathbf{a}_1 + l_2N_2\mathbf{a}_2 + l_3N_3\mathbf{a}_3\}) = P(\{\mathbf{1}|\mathbf{t}_\mathbf{n}\})$$

for any lattice vector $\mathbf{t}_\mathbf{n}$ and any set of integers l_1, l_2 and l_3, so that *only* $N = N_1N_2N_3$ of these operators are *distinct*. The set of distinct operators may be taken to be $P(\{\mathbf{1}|n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3\})$ with

$$0 \leq n_j < N_j,\ j = 1, 2, 3. \tag{7.4}$$

Moreover, as $P(\{\mathbf{1}|N_j\mathbf{a}_j\}) = P(\{\mathbf{1}|\mathbf{a}_j\})^{N_j}$, it follows from Equation (7.3) that

$$P(\{\mathbf{1}|\mathbf{a}_j\})^{N_j} = P(\{\mathbf{1}|\mathbf{0}\}),\ j = 1, 2, 3. \tag{7.5}$$

Thus this set of distinct operators forms a *finite* group $\mathcal{T}$ of order $N = N_1N_2N_3$. Henceforth this group $\mathcal{T}$ will be used in place of the infinite group of pure primitive translations $\mathcal{T}^\infty$.

Incidentally, as it remains true that

$$P(\{\mathbf{1}|\mathbf{t_n}\})\,P(\{\mathbf{1}|\mathbf{t_{n'}}\}) = P(\{\mathbf{1}|\mathbf{t_n}\}\{\mathbf{1}|\mathbf{t_{n'}}\})$$

for any two lattice vectors $\mathbf{t_n}$ and $\mathbf{t_{n'}}$ of a lattice, the mapping $\phi(\{\mathbf{1}|\mathbf{t_n}\}) = P(\{\mathbf{1}|\mathbf{t_n}\})$ is a homomorphic mapping of $\mathcal{T}^\infty$ onto $\mathcal{T}$. The kernel $\mathcal{K}$ of this mapping is the infinite set of pure primitive translations of the form $\{\mathbf{1}|l_1N_1\mathbf{a}_1 + l_2N_2\mathbf{a}_2 + l_3N_3\mathbf{a}_3\}$, where l_1, l_2 and l_3 are any set of integers.

3 Irreducible representations of the group $\mathcal{T}$ of pure primitive translations and Bloch's Theorem

As the group $\mathcal{T}$ is a finite Abelian group of order $N = N_1N_2N_3$, it possesses N inequivalent irreducible representations, all of which are one-dimensional (see Chapter 5, Section 6). These are easily found, for $\mathcal{T}$ is isomorphic to the direct product of three cyclic groups.

Consider a particular one-dimensional irreducible representation $\mathbf{\Gamma}$ of $\mathcal{T}$ and suppose that $\mathbf{\Gamma}(\{\mathbf{1}|\mathbf{a}_j\}) = [c_j]$, for $j = 1, 2, 3$. Then, from Equation (7.5), it follows that

$$c_j^{N_j} = 1, \tag{7.6}$$

so that

$$c_j = \exp(-2\pi i p_j/N_j),\ j = 1, 2, 3,$$

where p_j is an integer. As $\exp(-2\pi i(p_j + N_j)/N_j) = \exp(-2\pi i p_j/N_j)$, there are only N_j *different* values of c_j allowed by Equation (7.6) and each of these, by convention, may be taken to correspond to a p_j having one of the values $0, 1, 2, \ldots, N_j - 1$. Then

$$\mathbf{\Gamma}(\{\mathbf{1}|n_j\mathbf{a}_j\}) = [\exp(-2\pi i p_j n_j/N_j)]$$

and hence

$$\mathbf{\Gamma}(\{\mathbf{1}|\mathbf{t_n}) = [\exp(-2\pi i\{(p_1n_1/N_1) + (p_2n_2/N_2) + (p_3n_3/N_3)\})], \tag{7.7}$$

where $\mathbf{t_n} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$. There are $N = N_1N_2N_3$ sets of integers (p_1, p_2, p_3) allowed by the above convention which can be used to label the N different irreducible representations of $\mathcal{T}$.

Equation (7.7) can be simplified and given a simple geometric interpretation by introducing the following notation. Define the "basic lattice vectors of the reciprocal lattice" $\mathbf{b}_1, \mathbf{b}_2$ and $\mathbf{b}_3$ by

$$\mathbf{a}_j.\mathbf{b}_k = 2\pi\delta_{jk},\ j, k = 1, 2, 3, \tag{7.8}$$

so that, explicitly,

$$\mathbf{b}_1 = 2\pi \mathbf{a}_2 \wedge \mathbf{a}_3 / \{\mathbf{a}_1.(\mathbf{a}_2 \wedge \mathbf{a}_3)\}, \tag{7.9}$$

with similar expressions for $\mathbf{b}_2$ and $\mathbf{b}_3$. Then define the so-called "allowed $\mathbf{k}$-vectors" by

$$\mathbf{k} = k_1\mathbf{b}_1 + k_2\mathbf{b}_2 + k_3\mathbf{b}_3, \tag{7.10}$$

where $k_j = p_j/N_j$. Thus

$$\mathbf{k}.\mathbf{t_n} = 2\pi i\{(p_1 n_1/N_1) + (p_2 n_2/N_2) + (p_3 n_3/N_3)\},$$

so that Equation (7.7) becomes

$$\mathbf{\Gamma^k}(\{\mathbf{1}|\mathbf{t_n}\}) = [\exp(-i\mathbf{k}.\mathbf{t_n})], \tag{7.11}$$

where the N irreducible representations are now labelled by the allowed $\mathbf{k}$-vectors.

Suppose that $\phi_1^{\mathbf{k}}(\mathbf{r})$ is a basis function transforming as the first (and only) row of $\mathbf{\Gamma^k}$. Then, by Equations (1.26) and (7.11),

$$P(\{\mathbf{1}|\mathbf{t_n}\})\phi_1^{\mathbf{k}}(\mathbf{r}) = \mathbf{\Gamma^k}(\{\mathbf{1}|\mathbf{t_n}\})\phi_1^{\mathbf{k}}(\mathbf{r}) = \exp(-i\mathbf{k}.\mathbf{t_n})\phi_1^{\mathbf{k}}(\mathbf{r}). \tag{7.12}$$

However, by Equation (1.17),

$$P(\{\mathbf{1}|\mathbf{t_n}\})\phi_1^{\mathbf{k}}(\mathbf{r}) = \phi_1^{\mathbf{k}}(\{\mathbf{1}|\mathbf{t_n}\}^{-1}\mathbf{r}) = \phi_1^{\mathbf{k}}(\mathbf{r} - \mathbf{t_n}),$$

so that

$$\phi_1^{\mathbf{k}}(\mathbf{r} - \mathbf{t_n}) = \exp(-i\mathbf{k}.\mathbf{t_n})\phi_1^{\mathbf{k}}(\mathbf{r}).$$

Thus

$$\phi_1^{\mathbf{k}}(\mathbf{r}) = \exp(i\mathbf{k}.\mathbf{r})u_{\mathbf{k}}(\mathbf{r}), \tag{7.13}$$

where $u_{\mathbf{k}}(\mathbf{r})$ is a function that has the periodicity of the lattice, that is, $u_{\mathbf{k}}(\mathbf{r} - \mathbf{t_n}) = u_{\mathbf{k}}(\mathbf{r})$ for any lattice vector $\mathbf{t_n}$.

Equation (7.13) is the statement of the theorem of Bloch (1928) in its usual form, for electronic energy eigenfunctions must be basis functions of the irreducible representations $\mathbf{\Gamma^k}$ of $\mathcal{T}$. A function of the form in Equation (7.13) is therefore called a "Bloch function". The corresponding energy eigenvalue may be denoted by $\epsilon(\mathbf{k})$, so that

$$H(\mathbf{r})\phi_1^{\mathbf{k}}(\mathbf{r}) = \epsilon(\mathbf{k})\phi_1^{\mathbf{k}}(\mathbf{r}). \tag{7.14}$$

The notation for basis functions here follows the standard practice in which the irreducible representation is specified by a superscript (or set of superscripts) and the rows by a subscript (or set of subscripts). In particular, the wave vector $\mathbf{k}$ appears as a superscript with this convention. However, it should be pointed out that in most of the solid state literature $\mathbf{k}$ is written as a subscript, so that $\phi_1^{\mathbf{k}}(\mathbf{r})$ would be written as $\phi_{\mathbf{k}}(\mathbf{r})$ and Equation (8.20) would become $H(\mathbf{r})\phi_{\mathbf{k}}(\mathbf{r}) = \epsilon(\mathbf{k})\phi_{\mathbf{k}}(\mathbf{r})$.

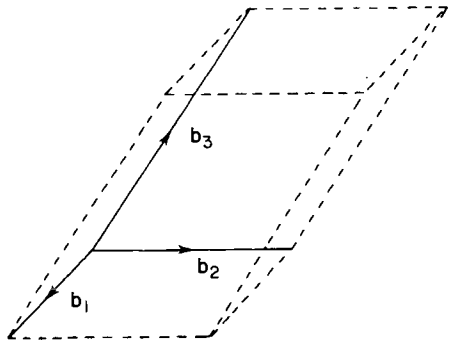

Figure 7.4: The basic parallelepiped of **k**-space.

4 Brillouin zones

The set of lattice vectors of the reciprocal lattice is defined by

$$\mathbf{K_m} = m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3, \tag{7.15}$$

where $\mathbf{m} = (m_1, m_2, m_3)$, m_1, m_2 and m_3 are integers, and $\mathbf{b}_1$, $\mathbf{b}_2$ and $\mathbf{b}_3$ are the basic lattice vectors of the reciprocal lattice defined by Equation (7.8). They have the property that

$$\exp(i\mathbf{K_m}.\mathbf{t_n}) = 1 \tag{7.16}$$

for any $\mathbf{K_m}$ and $\mathbf{t_n}$. It is useful to note that

$$\sum_{\mathbf{t_n}} \exp(i\mathbf{k}.\mathbf{t_n}) = \begin{cases} N, & \text{if } \mathbf{k} = \mathbf{K_m}, \\ 0, & \text{if } \mathbf{k} \neq \mathbf{K_m}, \end{cases} \tag{7.17}$$

where the sum is over all the lattice vectors of one basic block of Section 2, this result being a consequence of the fact that the left-hand side is a product of three simple geometric series. Similarly,

$$\sum_{\mathbf{k}} \exp(-i\mathbf{k}.\mathbf{t_n}) = \begin{cases} N, & \text{if } \mathbf{t_n} = \mathbf{0}, \\ 0, & \text{if } \mathbf{t_n} \neq \mathbf{0}, \end{cases}$$

the sum being over all allowed **k**-vectors.

In Section 3, N irreducible representations of $\mathcal{T}$ were found and described by the allowed **k**-vectors (Equation (7.10)). These **k**-vectors can be imagined as being plotted in the so-called "**k**-space" or "reciprocal space" defined by the reciprocal lattice vectors. The allowed **k**-vectors lie on a very fine lattice (defined by Equation (7.10)) within and upon three faces of the parallelepiped having edges $\mathbf{b}_1$, $\mathbf{b}_2$ and $\mathbf{b}_3$ that is shown in Figure 7.4.

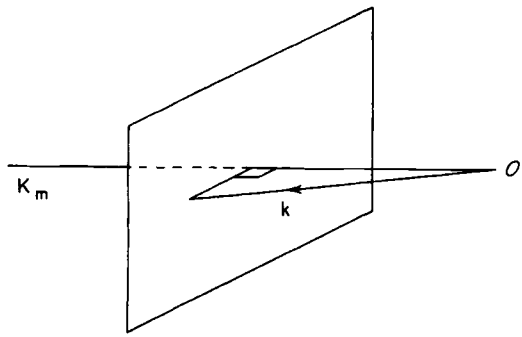

Figure 7.5: Construction of a Brillouin zone boundary.

It is, however, more convenient to replot the allowed **k**-vectors into a more symmetrical region of **k**-space surrounding the point $\mathbf{k} = \mathbf{0}$. To do this consider the equation ,

$$\mathbf{k}' = \mathbf{k} + \mathbf{K_m}, \tag{7.18}$$

where $\mathbf{K_m}$ is a reciprocal lattice vector. Two vectors **k** and **k**′ satisfying Equation (7.18) are said to be "equivalent", because $\exp(-i\mathbf{k}'.\mathbf{t_n}) = \exp(-i\mathbf{k}.\mathbf{t_n})$ by Equation (7.16), and hence

$$\mathbf{\Gamma}^{\mathbf{k}'}(\{\mathbf{1}|\mathbf{t_n}\}) = \mathbf{\Gamma}^{\mathbf{k}}(\{\mathbf{1}|\mathbf{t_n}\})$$

for every $\{\mathbf{1}|\mathbf{t_n}\}$ of $\mathcal{T}$. Thus the irreducible representation described by **k** could equally be described by **k**′. The more symmetrical region of **k**-space is called the "Brillouin zone" (or sometimes the "first Brillouin zone"), and it is defined to consist of all those points of **k**-space that lie closer to $\mathbf{k} = \mathbf{0}$ than to any other reciprocal lattice points. Its boundaries are therefore the planes that are the perpendicular bisectors of the lines joining the point $\mathbf{k} = \mathbf{0}$ to the nearer reciprocal lattice points, the plane bisecting the line from $\mathbf{k} = \mathbf{0}$ to $\mathbf{k} = \mathbf{K_m}$ having the equation

$$\mathbf{k}.\mathbf{K_m} = \frac{1}{2}|\mathbf{K_m}|^2,$$

as is clear from Figure 7.5. For some lattices, such as the body-centred cubic lattice Γ_c^v, only *nearest* neighbour reciprocal lattice points are involved in the construction of the Brillouin zone, but for others, such as the face-centred cubic lattice Γ_c^f, *next-nearest* neighbours are involved as well. The irreducible representations of $\mathcal{T}$ then correspond to a very fine lattice of points inside the Brillouin zone and on one half of its surface.

The mapping of the parallelepiped of Figure 7.4 into the Brillouin zone can be quite complicated because different regions of the parallelepiped are mapped using different reciprocal lattice vectors. The following two-dimensional example shown in Figure 7.6 of a square lattice demonstrates

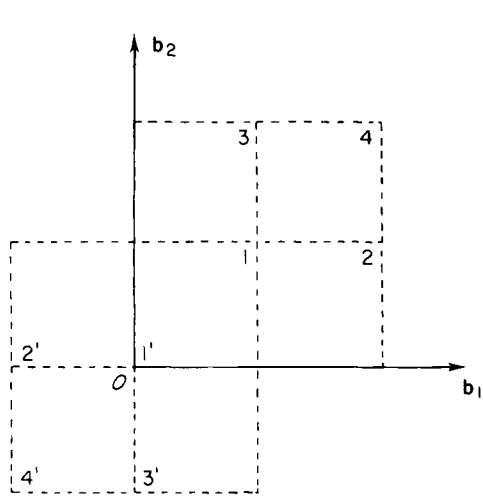

Figure 7.6: Construction of a two-dimensional Brillouin zone.

this clearly. In this example the analogue of the three-dimensional parallelepiped of Figure 7.5 is the square with sides $\mathbf{b}_1$ and $\mathbf{b}_2$, which consists of four regions 1, 2, 3 and 4, and the analogue of the Brillouin zone is the square having $\mathbf{k} = \mathbf{0}$ at its centre, which consists of the four regions $1'$, $2'$, $3'$ and $4'$. The region 1 is mapped into $1'$ by $\mathbf{K}_{(0,0,0)} = \mathbf{0}$, 2 is mapped into $2'$ by $\mathbf{K}_{(-1,0,0)} = -\mathbf{b}_1$, 3 is mapped into $3'$ by $\mathbf{K}_{(0,-1,0)} = -\mathbf{b}_2$, and 4 is mapped into $4'$ by $\mathbf{K}_{(-1,-1,0)} = -\mathbf{b}_1 - \mathbf{b}_2$.

By construction, the volume of the Brillouin zone is the same as that of the parallelepiped from which it is formed, namely $\mathbf{b}_1.(\mathbf{b}_2 \wedge \mathbf{b}_3)$. It follows from Equation (7.9) that this is equal to $(2\pi)^3/\{\mathbf{a}_1.(\mathbf{a}_2 \wedge \mathbf{a}_3)\}$, where $\mathbf{a}_1.(\mathbf{a}_2 \wedge \mathbf{a}_3)$ is the volume of the parallelepiped whose sides are $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$.

For the simple cubic lattice Γ_c, the basic lattice vectors of the reciprocal lattice obtained from Table 7.1 and Equation (7.9) are

$$\mathbf{b}_1 = (2\pi/a)(1,0,0),\ \mathbf{b}_2 = (2\pi/a)(0,1,0),\ \mathbf{b}_3 = (2\pi/a)(0,0,1).$$

The Brillouin zone is given in Figure 7.7. The position vectors of the "symmetry points" are as follows: for Γ, $\mathbf{k} = (0,0,0)$; for X, $\mathbf{k} = (\pi/a)(0,0,1)$; for M, $\mathbf{k} = (\pi/a)(0,1,1)$; and for R, $\mathbf{k} = (\pi/a)(1,1,1)$. The significance of the term "symmetry point" will be explained in Section 7. The notation is that of Bouckaert *et al.* (1936).

Similarly, for the body-centred cubic lattice Γ_c^v the basic lattice vectors of the reciprocal lattice are

$$\mathbf{b}_1 = (2\pi/a)(1,0,1),\ \mathbf{b}_2 = (2\pi/a)(0,1,-1),\ \mathbf{b}_3 = (2\pi/a)(1,-1,0),$$

the Brillouin zone being shown in Figure 7.8. The position vectors of the symmetry points are as follows: for Γ, $\mathbf{k} = (0,0,0)$; for H, $\mathbf{k} = (\pi/a)(0,0,2)$;

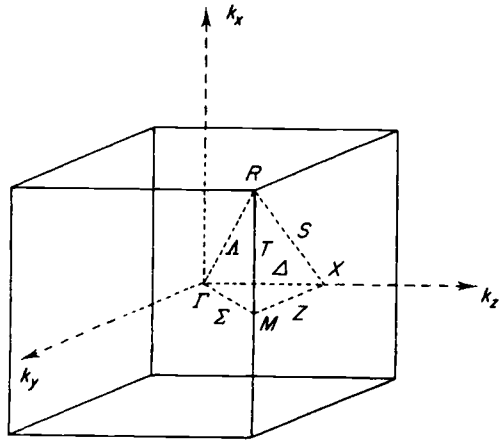

Figure 7.7: Brillouin zone corresponding to the simple cubic lattice Γ_c.

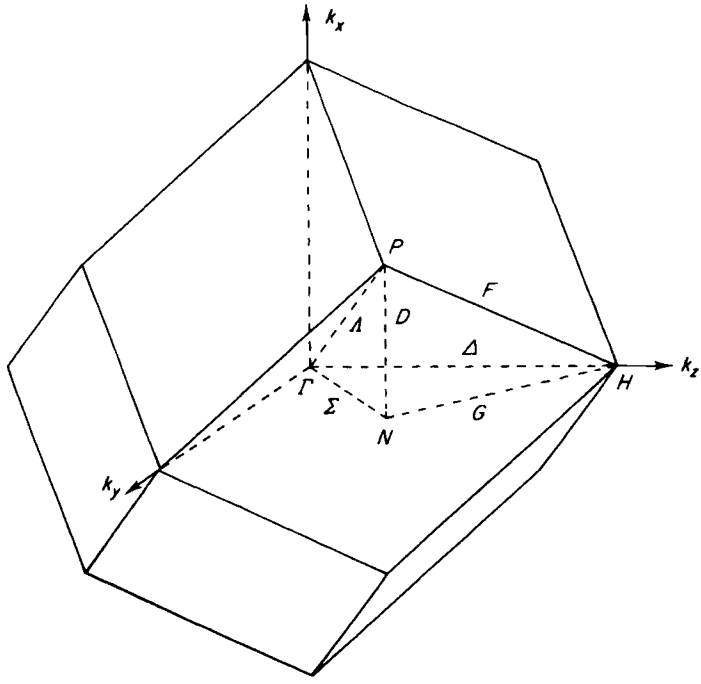

Figure 7.8: Brillouin zone corresponding to the body-centred cubic lattice Γ_c^v.

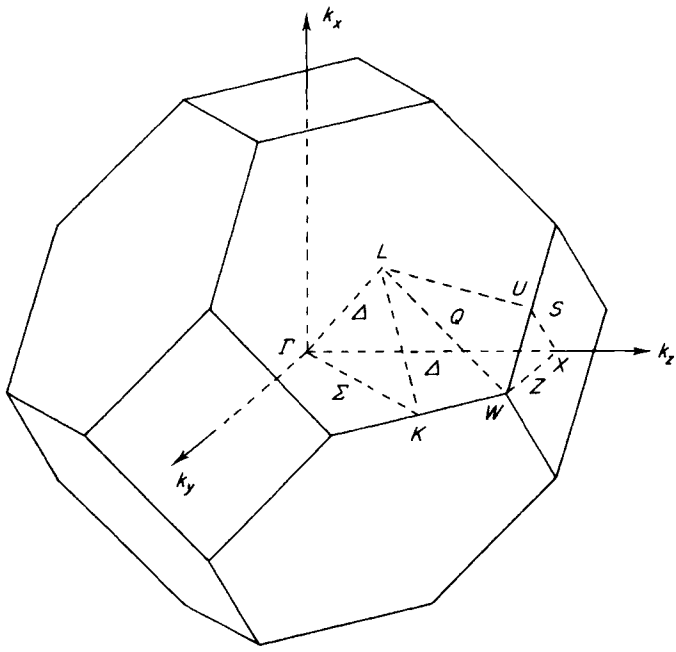

Figure 7.9: Brillouin zone corresponding to the face-centred cubic lattice Γ_c^f.

for N, $\mathbf{k} = (\pi/a)(0,1,1)$; and for P, $\mathbf{k} = (\pi/a)(1,1,1)$, the notation being that of Bouckaert *et al.* (1936).

Finally, for the face-centred cubic lattice Γ_c^f the basic lattice vectors of the reciprocal lattice are

$$\mathbf{b}_1 = (2\pi/a)(1,1,-1),\ \mathbf{b}_2 = (2\pi/a)(-1,1,1),\ \mathbf{b}_3 = (2\pi/a)(1,-1,1).$$

The Brillouin zone is given in Figure 7.9, the position vectors of the points indicated (in the notation of Bouckaert *et al.* (1936)) being: for Γ, $\mathbf{k} = (0,0,0)$; for K, $\mathbf{k} = (\pi/a)(0,\frac{3}{2},\frac{3}{2})$; for L, $\mathbf{k} = (\pi/a)(1,1,1)$; for U, $\mathbf{k} = (\pi/a)(\frac{1}{2},\frac{1}{2},2)$; for W, $\mathbf{k} = (\pi/a)(0,1,2)$; and for X, $\mathbf{k} = (\pi/a)(0,0,2)$.

The Brillouin zones corresponding to the other eleven Bravais lattices may be found in the review article by Koster (1957).

5 Electronic energy bands

The set of energy eigenvalues corresponding to an allowed $\mathbf{k}$-vector may be denoted by $\epsilon_1(\mathbf{k}), \epsilon_2(\mathbf{k}), \ldots$, with the convention that

$$\epsilon_n(\mathbf{k}) \leq \epsilon_{n+1}(\mathbf{k}) \tag{7.19}$$

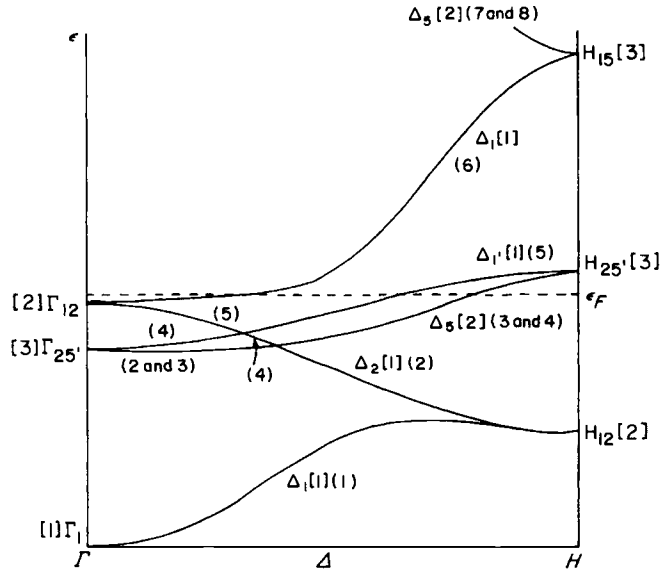

Figure 7.10: Part of the electronic energy band structure of iron.

for all $n = 1, 2, \ldots$. The set of energy eigenvalues $\epsilon_n(\mathbf{k})$ corresponding to a particular n are said to form the "nth energy band" and the set of energy bands is said to constitute the electronic energy band "structure".

To visualize the energy band structure, it is convenient to consider, one at a time, the axes of the Brillouin zone that join the symmetry points, and for each allowed $\mathbf{k}$-vector on each axis to plot the energy eigenvalues $\epsilon_n(\mathbf{k})$. Two typical examples are shown in Figures 7.10 and 7.11, which give the energy levels along the axis Δ for iron (as calculated by Wood (1962)) and silicon (as calculated by Chelikowsky and Cohen (1976)), the lattices being the body-centred cubic and face-centred cubic respectively. The number in curved brackets gives the band index n, as defined in Expression (7.19) and the number in square brackets indicates the degeneracy of the corresponding eigenvalue. (The occurrence of degenerate eigenvalues is a consequence of the rotational symmetry, which is being neglected in this section but which will be investigated in Sections 7 and 8, where the other symbols will also be explained.)

The positive integers N_1, N_2 and N_3 introduced in Equations (7.2) are arbitrarily large, and it is frequently convenient to consider the limiting case in which they tend to infinity. The allowed $\mathbf{k}$-vectors can then take *all* values inside the Brillouin zone and on half of its surface, and the $\epsilon_n(\mathbf{k})$ are continuous functions of $\mathbf{k}$ for each n. Moreover, $\mathrm{grad}_{\mathbf{k}}\epsilon_n(\mathbf{k})$ are also continuous functions of $\mathbf{k}$, except possibly at points where two bands touch. The plots in Figures 7.10 and 7.11 are made for this limiting case.

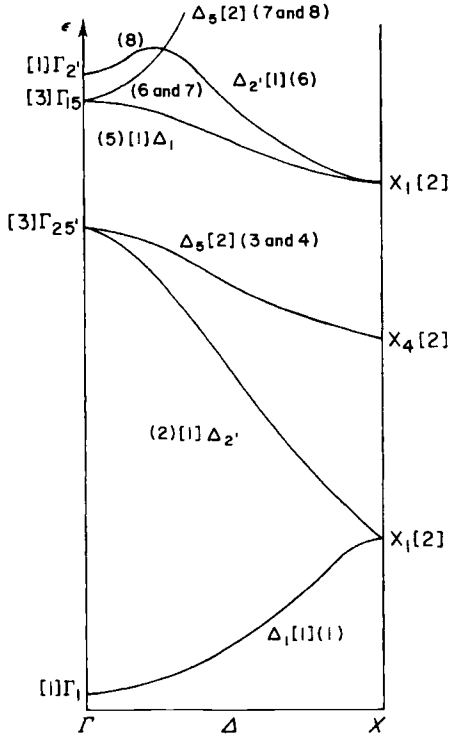

Figure 7.11: Part of the electronic energy band structure of silicon.

In the "single-particle" approximation (see Chapter 1, Section 3(a)), the Pauli exclusion principle implies that no two electrons can "occupy" the same one-electron state. With the present neglect of spin-dependent terms, such a state is specified by an allowed **k**-vector, a band index n, and a spin quantum number that can take one of two possible values. It follows that each energy level $\epsilon_n(\mathbf{k})$ can "hold" *two* electrons and hence each energy band can hold $2N$ electrons. If there are V valence or conduction electrons per atom and S atoms per lattice point of the crystal, there will be NVS valence or conduction electrons in each large basic block of the crystal (in the sense of Section 2), which will therefore require the equivalent of $\frac{1}{2}VS$ bands to hold them.

In the ground state of the system all the energy levels will be doubly occupied up to a certain energy ϵ_F, the "Fermi energy", and all levels above this energy will be unoccupied. The surface in k-space defined by

$$\epsilon_n(\mathbf{k}) = \epsilon_F$$

is called the "Fermi surface". The distribution of energy levels near the Fermi energy largely determines the electronic properties of a solid. If one and only one band contains the Fermi energy, and all others are entirely above it or below it, then the Fermi surface merely consists of one sheet. If no band

contains the Fermi energy, as happens for insulators and semiconductors, there is no Fermi surface. In all other cases the Fermi surface consists of several sheets, to visualize which one considers a number of identical Brillouin zones, with one zone for each band. A full band corresponds to a full Brillouin zone, but a partially occupied band corresponds to a partially occupied Brillouin zone and hence to a sheet of the Fermi surface in that zone.

As an example, consider body-centred cubic iron for which $S = 1$ and $V = 8$, so that the equivalent of four complete bands are needed to hold the valence electrons. The Fermi energy ϵ_F is shown in Figure 7.10 and is clearly consistent with this. Bands 3, 4, 5 and 6 are partially occupied, giving rise to four sheets in the Fermi surface.

For silicon $V = 4$ and $S = 2$, so that again four bands (or their equivalent) are required to hold the valence electrons. However, in this case there is no overlap between the 4th and 5th bands, so that the Fermi energy lies between the X_1 and $\Gamma_{25'}$ levels of Figure 7.11. There are therefore four completely filled bands and no Fermi surface.

6 Survey of the crystallographic space groups

Consider an infinite crystalline solid for which the equilibrium positions of the nuclei are given by Equation (7.1). The set of all coordinate transformations that map the set of equilibrium positions into itself forms an infinite group $\mathcal{G}^\infty$ that is known as a "crystallographic space group". Clearly $\mathcal{G}^\infty$ contains as a subgroup the infinite group of pure primitive translations $\mathcal{T}^\infty$ of the relevant lattice, but contains no other pure translations.

If $\{\mathbf{R}|\mathbf{t}\}$ is a member of the space group $\mathcal{G}^\infty$ and $\mathbf{t_n}$ is any lattice vector of its lattice, then $\mathbf{Rt_n}$ must also be a lattice vector. (This follows because (by Equations (1.7) and (1.8)) $\{\mathbf{R}|\mathbf{t}\}\{\mathbf{1}|\mathbf{t_n}\}\{\mathbf{R}|\mathbf{t}\}^{-1} = \{\mathbf{1}|\mathbf{Rt_n}\}$, so that $\{\mathbf{1}|\mathbf{Rt_n}\}$ must be a member of $\mathcal{G}^\infty$ and, being a pure translation, must be a primitive translation. Thus the set of all rotational parts $\mathbf{R}$ of the space group operations $\{\mathbf{R}|\mathbf{t}\}$ form a subgroup $\mathcal{G}_0$ of the maximal point group $\mathcal{G}_0^{max}$ of its crystal lattice (though $\mathcal{G}_0$ need not be a proper subgroup of $\mathcal{G}_0^{max}$). $\mathcal{G}_0$ is known as the "point group of the space group".

Detailed investigations show that the only possible proper rotations of $\mathcal{G}_0$ are through multiples of $2\pi/6$ or $2\pi/4$, and the only possible improper rotations are products of these proper rotations with the spatial inversion operator. Consequently $\mathcal{G}_0$ is always a finite group, and must be one of the 32 crystallographic point groups that are specified in detail in Appendix C. (Of course these restrictions disappear if the requirement of translational symmetry is abandoned. Consequently, for a "quasicrystal", which has no such translational symmetry, it is possible to have other rotations as well, including, in particular, the proper rotations through $2\pi/5$.)

Space groups having the same point group $\mathcal{G}_0$ are said to belong to the same "crystal class", so there are 32 different crystal classes. In the classification of space groups by Schönfliess (1923), each space group is denoted by the

Schönfliess symbol for its point group $\mathcal{G}_0$, together with a superscript. Thus, for example, the space groups for crystals possessing the cubic Bravais lattices Γ_c, Γ_c^v and Γ_c^f, and having only nuclei at the lattice points, all have O_h as point group, and are denoted by O_h^1, O_h^9 and O_h^5 respectively. Similarly, the space group of the diamond structure, which also has the Bravais lattice Γ_c^f and point group O_h but which has two nuclei per lattice site, is denoted by O_h^7. As will be seen, the assignment of superscripts by Schönfliess is rather arbitrary. An alternative that is more explicit but more complicated is the "international notation" (see Henry and Lonsdale 1965, Shubnikov and Koptsik 1974, Burns and Glazer 1978).

To every rotation $\{\mathbf{R}|\mathbf{0}\}$ of $\mathcal{G}_0$ there exists a vector $\boldsymbol{\tau}_\mathbf{R}$ which is such that $\{\mathbf{R}|\boldsymbol{\tau}_\mathbf{R}+\mathbf{t_n}\}$ is a member of $\mathcal{G}^\infty$ for every lattice vector $\mathbf{t_n}$ of the lattice. Moreover, $\boldsymbol{\tau}_\mathbf{R}$ is unique (up to a lattice vector), as if $\{\mathbf{R}|\boldsymbol{\tau}_\mathbf{R}\}$ and $\{\mathbf{R}|\boldsymbol{\tau}'_\mathbf{R}\}$ are both members of $\mathcal{G}^\infty$ then so must be $\{\mathbf{R}|\boldsymbol{\tau}_\mathbf{R}\}\{\mathbf{R}|\boldsymbol{\tau}'_\mathbf{R}\}^{-1}=\{\mathbf{1}|\boldsymbol{\tau}_\mathbf{R}-\boldsymbol{\tau}'_\mathbf{R}\}$, which, being a pure translation, is bound to be a primitive translation, so that $\boldsymbol{\tau}'_\mathbf{R}=\boldsymbol{\tau}_\mathbf{R}+\mathbf{t_n}$ for some $\mathbf{t_n}$. For definiteness it will be assumed henceforth that $\boldsymbol{\tau}_\mathbf{R}$ is always chosen so that $\boldsymbol{\tau}_\mathbf{R}=q_1\mathbf{a}_1+q_2\mathbf{a}_2+q_3\mathbf{a}_3$ with $0\le q_j<1$, $j=1,2,3$.

If $\boldsymbol{\tau}_\mathbf{R}=\mathbf{0}$ for every $\{\mathbf{R}|\mathbf{0}\}\in\mathcal{G}_0$, then $\mathcal{G}^\infty$ is said to be a "symmorphic" space group. That is, for a symmorphic space group *every* transformation is of the form $\{\mathbf{R}|\mathbf{t_n}\}$, the translational part *always* being a *lattice vector*. Obviously, if $\mathcal{G}^\infty$ is symmorphic, then $\mathcal{G}_0$ is a subgroup of $\mathcal{G}^\infty$. Only 73 of the 230 crystallographic space groups in $\mathbb{R}^3$ are symmorphic. Important examples include the cubic space groups O_h^1, O_h^5 and O_h^9. However, if $\mathcal{G}^\infty$ is non-symmorphic, then for some $\{\mathbf{R}|\mathbf{0}\}\in\mathcal{G}_0$ there exists a *non-zero* $\boldsymbol{\tau}_\mathbf{R}$. Thus, if $\mathcal{G}^\infty$ is non-symmorphic, $\mathcal{G}_0$ is not a subgroup of $\mathcal{G}^\infty$.

If a crystal has nuclei of only one species and their equilibrium positions lie only at the lattice points of a Bravais lattice, then the corresponding space group is symmorphic. The same is true if the crystal has more than one species of nuclei and if the arrays of nuclei of each species each form a Bravais lattice. (This is only possible if there is only one nucleus of each species per lattice site.) By contrast, non-symmorphic space groups are associated with crystals in which there are more than one nuclei of a given species per lattice site.

Only the representation theory of *symmorphic* space groups will be considered in Section 7. For a description of the corresponding theory for non-symmorphic space groups see, for example, Chapter 9, Section 3, of Cornwell (1984).

A complete description of all 230 space groups may be found in the *International Tables for X-ray Crystallography* (Henry and Lonsdale 1965), which employ both the Schönfliess and international notations. (A simple prescription for determining the symmetry elements of a space group from the "general position" listed in the International Tables has been given by Wondratschek and Neubuser (1967).) Another complete specification that is particularly clear and thorough has been given by Shubnikov and Koptsik (1974). A further clear and comprehensive description of the crystallographic space

groups has been given by Burns and Glazer (1978). Lists of the space groups to which elements and compounds belong have been compiled by Wyckoff (1963,1964,1965) and by Donnay and Nowacki (1954).

The effect of imposing Born cyclic boundary conditions is to replace the infinite space group $\mathcal{G}^\infty$ by a *finite* group $\mathcal{G}$. As a preliminary, let $N_1 = N_2 = N_3$, where N_1, N_2, N_3 are as defined in Equations (7.2). (For every $\{\mathbf{R}|\mathbf{0}\} \in \mathcal{G}_0$ this ensures that $\mathbf{R}(N_j\mathbf{a}_j) = l_1N_1\mathbf{a}_1 + l_2N_2\mathbf{a}_2 + l_3N_3\mathbf{a}_3$ for some *integers* l_1, l_2 and l_3 and each $j = 1, 2, 3$.)

Thus, in the symmorphic case, $\mathcal{G}$ may be defined to be the group of operators $P(\{\mathbf{R}|\mathbf{t_n}\})$ for all $\{\mathbf{R}|\mathbf{0}\} \in \mathcal{G}_0$ and all lattice vectors $\mathbf{t_n}$ of the *finite* group $\mathcal{T}$ with Equation (7.5) applied. Then $\mathcal{G}$ has order g_0N, where g_0 and N are the orders of $\mathcal{G}_0$ and $\mathcal{T}$ respectively.

As it remains true that $P(\{\mathbf{R}|\mathbf{t}\})P(\{\mathbf{R}'|\mathbf{t}'\}) = P(\{\mathbf{R}|\mathbf{t}\}\{\mathbf{R}'|\mathbf{t}'\})$ for every $\{\mathbf{R}|\mathbf{t}\}$ and $\{\mathbf{R}'|\mathbf{t}'\}$ of $\mathcal{G}$, the mapping $\Phi(\{\mathbf{R}|\mathbf{t}\}) = P(\{\mathbf{R}|\mathbf{t}\})$ is a homomorphic mapping of $\mathcal{G}^\infty$ onto $\mathcal{G}$. The kernel $\mathcal{K}$ of this mapping is again the infinite set of pure primitive translations of the form $\{\mathbf{1}|l_1N_1\mathbf{a}_1 + l_2N_2\mathbf{a}_2 + l_3N_3\mathbf{a}_3\}$, where l_1, l_2 and l_3 are any set of integers.

With the inner product defined as in Section 2, i.e. so that it involves an integral over just one basic block of the crystal, B, the operators $P(\{\mathbf{R}|\mathbf{t}\})$ retain the unitary property of Equation (1.20), provided all the functions on which they act satisfy the Born cyclic boundary conditions (Equations (7.2)).

The following sections will be devoted to the study of the representations of the finite symmorphic space groups $\mathcal{G}$ and of their consequences. In this context no confusion will be caused if the Schönfliess or international notations are applied to the finite space groups as well as to the corresponding infinite groups.

An identity that is worth noting is

$$\mathbf{t}.(\mathbf{Rk}) = (\mathbf{R}^{-1}\mathbf{t}).\mathbf{k}, \tag{7.20}$$

which is valid for *any* rotation $\mathbf{R}$ and *any* vectors $\mathbf{t}$ and $\mathbf{k}$. This follows because $\mathbf{R}$ is a 3×3 orthogonal matrix (see Chapter 1, Section 2((a)), so that

$$\mathbf{t}.(\mathbf{Rk}) = \sum_{i=1}^{3} t_i(\mathbf{Rk})_i = \sum_{i,j=1}^{3} t_iR_{ij}k_j = \sum_{i,j=1}^{3} (\mathbf{R}^{-1})_{ji}t_ik_j = (\mathbf{R}^{-1}\mathbf{t}).\mathbf{k}.$$

This implies that the reciprocal lattice (as defined in Section 4) has the *same* symmetry as the crystal lattice to which it belongs. This is shown by the following theorem.

Theorem I If $\{\mathbf{R}|\mathbf{0}\}$ of $\mathcal{G}_0$ and $\mathbf{K_m}$ is a lattice vector of the reciprocal lattice, then $\mathbf{RK_m}$ is also a lattice vector of the reciprocal lattice.

Proof Suppose that $\mathbf{RK_m}$ is *not* a lattice vector of the reciprocal lattice. Then there exists a lattice vector $\mathbf{t_n}$ of the crystal lattice that is such that $\exp\{i\mathbf{t_n}.(\mathbf{RK_m})\} \neq 1$. Thus, by Equation (7.20), $\exp\{i(\mathbf{R}^{-1}\mathbf{t_n}).\mathbf{K_m}\} \neq 1$.

However, $\{\mathbf{R}^{-1}|\mathbf{0}\}$ is a member of $\mathcal{G}_0$, so $\mathbf{R}^{-1}\mathbf{t_n}$ must be a lattice vector of the crystal lattice. Equation (7.16) then provides a contradiction.

7 Irreducible representations of symmorphic space groups

(a) Fundamental theorem on irreducible representations of symmorphic space groups

The first stage in the analysis of symmorphic space groups is to observe that they possess a particularly straightforward structure.

Theorem I If $\mathcal{G}$ is a *symmorphic* space group, then $\mathcal{G}$ is isomorphic to the semi-direct product $\mathcal{T}\textcircled{s}\mathcal{G}_0$.

Proof All that has to be verified is that the three requirements of the definition of Chapter 2, Section 7, are satisfied. Firstly, $\mathcal{T}$ is clearly an invariant subgroup of $\mathcal{G}$. Moreover $\mathcal{T}$ and $\mathcal{G}_0$ have only the identity in common. Finally, if $\mathcal{G}$ is symmorphic, every element of $\mathcal{G}$ is the product of a pure primitive translation of $\mathcal{T}$ with a pure rotation of $\mathcal{G}_0$.

As $\mathcal{T}$ is Abelian, the theory of induced representations given in Chapter 5, Section 7, can be applied to produce *all* the irreducible representations of $\mathcal{G}$. Moreover, all the "little groups" from which the irreducible representations of $\mathcal{G}$ are induced are subgroups of $\mathcal{G}_0$, and hence every "little group" is a crystallographic point group. As all the irreducible representations of the crystallographic point groups are known (and are listed in Appendix C), the irreducible representations of the space group $\mathcal{G}$ follow immediately.

In applying the results of the induced representation theory it is very helpful to re-cast some of the concepts in terms of the geometric picture of the Brillouin zone and its allowed $\mathbf{k}$-vectors developed in Section 4. The quantities that will now be introduced will be identified in the proof of the fundamental theorem with certain of the entities of the induced representation theory.

Definition $\mathcal{G}_0(\mathbf{k})$, *the point group of the allowed wave vector* $\mathbf{k}$
The point group $\mathcal{G}_0(\mathbf{k})$ is the subgroup of the point group $\mathcal{G}_0$ of the space group $\mathcal{G}$ that consists of all the rotations $\{\mathbf{R}|\mathbf{0}\}$ of $\mathcal{G}_0$ that rotate $\mathbf{k}$ into itself or an "equivalent" vector (in the sense of Equation (7.18)). That is, $\{\mathbf{R}|\mathbf{0}\}$ of $\mathcal{G}_0$ is a member of $\mathcal{G}_0(\mathbf{k})$ if there exists a lattice vector $\mathbf{K_m}$ of the reciprocal lattice (as defined in Equation (7.15)), which may be zero, such that

$$\mathbf{Rk} = \mathbf{k} + \mathbf{K_m}. \tag{7.21}$$

Let g_0 and $g_0(\mathbf{k})$ be the orders of $\mathcal{G}_0$ and $\mathcal{G}_0(\mathbf{k})$ respectively, and let $M(\mathbf{k})$

be defined by

$$M(\mathbf{k}) = g_0/g_0(\mathbf{k}). \tag{7.22}$$

Then (see Chapter 2, Section 4) $M(\mathbf{k})$ is always an *integer.*

Definition *General points, symmetry points, symmetry axes and symmetry planes of the Brillouin zone*
If $\mathcal{G}_0(\mathbf{k})$ is the trivial group consisting only of the identity transformation $\{\mathbf{1}|\mathbf{0}\}$, then $\mathbf{k}$ is said to be a "general point" of the Brillouin zone. If $\mathbf{k}$ is such that $\mathcal{G}_0(\mathbf{k})$ is a larger group than those corresponding to all neighbouring points of the Brillouin zone, then $\mathbf{k}$ is known as a "symmetry point". If all the points on a line or plane have the same non-trivial $\mathcal{G}_0(\mathbf{k})$, then this line or plane is said to be a "symmetry axis" or "symmetry plane".

It is easily shown that this list of definitions exhausts all the possible situations.

Example I *Symmetry points, axes and planes for the space group* O_h^9
The Brillouin zone of the body-centred cubic lattice Γ_c^v is shown in Figure 7.8. For the space group O_h^9 with this lattice the symmetry points are Γ, H, N and P, and the symmetry axes are Δ, Λ, Σ, D, F and G, and the symmetry planes are the planes containing two symmetry axes.

Example II *Symmetry points, axes and planes for the space group* O_h^5
The Brillouin zone of the face-centred cubic lattice Γ_c^v is given in Figure 7.9. For the space group O_h^5 with this lattice the symmetry points are Γ, L, W and X, the symmetry axes are Δ, Λ, Σ, Q, S and Z, and the symmetry planes are ΓKWX, ΓKL, ΓLUX and UWX. The point K is *not* a symmetry point because its $\mathcal{G}_0(\mathbf{k})$ is the same as that for the axis Σ that ends at K. For the same reason U is *not* a symmetry point. It should be noted also that $KLUW$ is not a symmetry plane. Finally, the lines LK, KW, LU and UW have only the symmetry of the symmetry planes to which they belong, so they are not regarded as symmetry axes.

Definition *The "star" of* $\mathbf{k}$
Let $\{\mathbf{R}_j|\mathbf{0}\}$, $j = 1, 2, \ldots, M(\mathbf{k})$, be a set of coset representatives for the decomposition of $\mathcal{G}_0$ into left cosets with respect to $\mathcal{G}_0(\mathbf{k})$ (see Chapter 2, Section 4). Then the set of $M(\mathbf{k})$ vectors $\mathbf{k}_j$ defined by $\mathbf{k}_j = \mathbf{R}_j\mathbf{k}$ $(j = 1, 2, \ldots, M(\mathbf{k}))$ is called the "star" of $\mathbf{k}$.

Of course any member of a left coset can be chosen to be the coset representative, but once a choice is made it should be adhered to. If $\{\mathbf{R}'_j|\mathbf{0}\} \in \{\mathbf{R}_j|\mathbf{0}\}\mathcal{G}_0(\mathbf{k})$, then there exists an element $\{\mathbf{R}|\mathbf{0}\}$ of $\mathcal{G}_0(\mathbf{k})$ such that $\mathbf{R}'_j = \mathbf{R}_j\mathbf{R}$. Then $\mathbf{R}'_j\mathbf{k} = \mathbf{R}_j(\mathbf{R}\mathbf{k}) = \mathbf{R}_j\mathbf{k} + \mathbf{R}_j\mathbf{K}_\mathbf{m}$ (by Equation (7.21)), so that $\mathbf{R}'_j\mathbf{k}$ is equivalent to $\mathbf{R}_j\mathbf{k}$, as $\mathbf{R}_j\mathbf{K}_\mathbf{m}$ is a reciprocal lattice vector. Thus a different choice of the coset representatives merely results in a set of vectors that are equivalent to those of the set $\mathbf{k}_1, \mathbf{k}_2, \ldots$. Consequently the star of $\mathbf{k}$

is unique up to equivalence. It is always convenient to choose $\mathbf{R}_1 = \mathbf{1}$, so that $\mathbf{k}_1 = \mathbf{k}$.

The fundamental theorem on the irreducible representations of a symmorphic space group can now be presented.

Theorem II Let $\mathbf{k}$ be any allowed $\mathbf{k}$-vector of the Brillouin zone and let $\{\mathbf{R}_j|\mathbf{0}\}$ $(j = 1, 2, \ldots, M(\mathbf{k}))$ be a set of coset representatives for the decomposition of $\mathcal{G}_0$ into left cosets with respect to $\mathcal{G}_0(\mathbf{k})$. Let $\mathbf{\Gamma}^p_{\mathcal{G}_0(\mathbf{k})}$ be a unitary irreducible representation of $\mathcal{G}_0(\mathbf{k})$, assumed to be of dimension d_p. Then there exists a corresponding unitary irreducible representation of the space group $\mathcal{G}$ of dimension $d_p M(\mathbf{k})$, which may be denoted by $\mathbf{\Gamma}^{\mathbf{k}p}$, such that

$$\Gamma^{\mathbf{k}p}(\{\mathbf{R}|\mathbf{t_n}\})_{kt,jr} = \begin{cases} \exp\{-i(\mathbf{R}_k\mathbf{k}).\mathbf{t_n}\}\, \Gamma^p_{\mathcal{G}_0(\mathbf{k})}(\{\mathbf{R}_k^{-1}\mathbf{R}\mathbf{R}_j|\mathbf{0}\})_{tr}, \\ \quad \text{if } \mathbf{R}_k^{-1}\mathbf{R}\mathbf{R}_j \in \mathcal{G}_0(\mathbf{k}), \\ 0, \text{ otherwise}, \end{cases} \tag{7.23}$$

for $j, k = 1, 2, \ldots, M(\mathbf{k})$, and $r, t = 1, 2, ..., d_p$. (Here each row and column is specified by a *pair* of indices.) Moreover, *all* the inequivalent irreducible representations of $\mathcal{G}$ may be obtained in this way by working through all the inequivalent irreducible representations of $\mathcal{G}_0(\mathbf{k})$ for all allowed $\mathbf{k}$-vectors that are in different stars.

Proof All that is required is to identify the concepts introduced above with those developed for induced representations in Chapter 5, Section 7. The required result is then an immediate consequence of Theorem II of Chapter 5, Section 7.

Theorem I above showed that $\mathcal{G}$ is isomorphic to $\mathcal{T}\textcircled{s}\mathcal{G}_0$, so the groups $\mathcal{A}$ and $\mathcal{B}$ can be identified with $\mathcal{T}$ and $\mathcal{G}_0$ respectively. As the characters of $\mathcal{T}$ are specified by the allowed $\mathbf{k}$-vectors and are given by Equation (7.11), the label q may be identified with $\mathbf{k}$. Thus with $A = \{\mathbf{1}|\mathbf{t_n}\}$

$$\chi^q_{\mathcal{A}}(A) = \exp(-i\mathbf{k}.\mathbf{t_n}). \tag{7.24}$$

With $B = \{\mathbf{R}|\mathbf{0}\}$, $BAB^{-1} = \{\mathbf{1}|\mathbf{R}\mathbf{t_n}\}$, so

$$\chi^q_{\mathcal{A}}(BAB^{-1}) = \exp\{-i\mathbf{k}.(\mathbf{R}\mathbf{t_n})\} = \exp\{-i(\mathbf{R}^{-1}\mathbf{k}).\mathbf{t_n}\}$$

(by Equation (7.20)). Thus Equation (5.43) implies that the subgroup $\mathcal{B}(q)$ of $\mathcal{B}$ is merely $\mathcal{G}_0(\mathbf{k})$, that is, *the* $\mathcal{G}_0(\mathbf{k})$ *are the "little groups"*. Clearly $b = g_0$, $b(q) = g_0(\mathbf{k})$, and $M(q) = M(\mathbf{k})$.

If $\{\mathbf{R}_j|\mathbf{0}\}$ $(j = 1, 2, \ldots, M(\mathbf{k}))$ are the coset representatives for the decomposition of $\mathcal{G}_0$ into *left* cosets with respect to $\mathcal{G}_0(\mathbf{k})$, then $\{\mathbf{R}_j|\mathbf{0}\}^{-1}$ $(j = 1, 2, \ldots, M(\mathbf{k}))$ may be taken as the coset representatives for the decomposition of $\mathcal{G}_0$ into *right* cosets with respect to $\mathcal{G}_0(\mathbf{k})$. (This follows because, if $\{\mathbf{R}_j|\mathbf{0}\}^{-1}$ and $\{\mathbf{R}_k|\mathbf{0}\}^{-1}$ belong to the same right coset, there exists an $\{\mathbf{R}|\mathbf{0}\}^{-1}$ of $\mathcal{G}_0$ such that $\{\mathbf{R}_k|\mathbf{0}\}^{-1} = \{\mathbf{R}|\mathbf{0}\}\{\mathbf{R}_j|\mathbf{0}\}^{-1}$. Then $\{\mathbf{R}_k|\mathbf{0}\} = \{\mathbf{R}_j|\mathbf{0}\}\{\mathbf{R}|\mathbf{0}\}^{-1}$, which implies that $\{\mathbf{R}_j|\mathbf{0}\}$ and $\{\mathbf{R}_k|\mathbf{0}\}$ belong to the same

left coset.) Thus the coset representatives B_j $(j = 1, 2, \ldots, M(q))$ for the decomposition of $\mathcal{B}$ into right cosets with respect to $\mathcal{B}(q)$ may be identified with $\{\mathbf{R}_j|\mathbf{0}\}^{-1}$ $(j = 1, 2, \ldots, M(\mathbf{k}))$.

Then, by Equations (5.44), (7.20) and (7.24), with $A = \{\mathbf{1}|\mathbf{t_n}\}$,

$$\chi_{\mathcal{A}}^{B_j(q)}(A) = \exp\{-i(\mathbf{R}_j\mathbf{k}).\mathbf{t_n}\}, \tag{7.25}$$

and Equations (5.47) reduce to Equations (7.23). Finally, the *orbit* of q is obviously merely the *star* of $\mathbf{k}$.

This theorem removes the need for an explicit display of the character table for $\mathcal{G}$, which would in any case be very difficult because of the vast number of irreducible representations that $\mathcal{G}$ possesses. All the information required about $\mathcal{G}$ on such things as basis functions and degeneracies is immediately provided by the theorem in terms of the corresponding quantities for crystallographic point groups, which are very easily obtained.

The character $\chi^{\mathbf{k}p}(\{\mathbf{R}|\mathbf{t_n}\})$ of $\{\mathbf{R}|\mathbf{t_n}\}$ in the irreducible representation $\mathbf{\Gamma}^{\mathbf{k}p}$ of $\mathcal{G}$ is given by

$$\chi^{\mathbf{k}p}(\{\mathbf{R}|\mathbf{t_n}\}) = \sum_j \exp\{-i(\mathbf{R}_j\mathbf{k}).\mathbf{t_n}\}\, \chi^p_{\mathcal{G}_0(\mathbf{k})}(\{\mathbf{R}_j^{-1}\mathbf{R}\mathbf{R}_j|\mathbf{0}\}), \tag{7.26}$$

where the sum is over all the coset representatives $\mathbf{R}_j$ such that $\{\mathbf{R}_j^{-1}\mathbf{R}\mathbf{R}_j|\mathbf{0}\}$ $\in \mathcal{G}_0(\mathbf{k})$ and where $\chi^p_{\mathcal{G}_0(\mathbf{k})}$ denotes the character of the irreducible representation $\mathbf{\Gamma}^p_{\mathcal{G}_0(\mathbf{k})}$ of $\mathcal{G}_0(\mathbf{k})$. (This follows immediately from Equation (5.48) using Equation (7.25).)

In applications the following properties of the basis functions of $\mathbf{\Gamma}^{\mathbf{k}p}$ of $\mathcal{G}_0(\mathbf{k})$ are useful.

Theorem III Let $\psi^{\mathbf{k}p}_{jr}(\mathbf{r})$ $(j = 1, 2, \ldots, M(\mathbf{k})$, and $r = 1, 2, \ldots, d_p)$ be a set of basis functions of the unitary irreducible representation $\mathbf{\Gamma}^{\mathbf{k}p}$ of the space group $\mathcal{G}$ defined by Equations (7.23). Then

(a) $\psi^{\mathbf{k}p}_{jr}(\mathbf{r})$ is a Bloch function with wave vector $\mathbf{R}_j\mathbf{k}$,

(b) the functions $\psi^{\mathbf{k}p}_{1r}(\mathbf{r})$ $(r = 1, 2, \ldots, d_p)$ form a basis for the unitary irreducible representation $\mathbf{\Gamma}^{\mathbf{k}p}$ of $\mathcal{G}_0(\mathbf{k})$, and

(c) $\psi^{\mathbf{k}p}_{jr}(\mathbf{r}) = P(\{\mathbf{R}_j|\mathbf{0}\})\psi^{\mathbf{k}p}_{1r}(\mathbf{r})$, for $j = 1, 2, \ldots, M(\mathbf{k})$.

Proof In the double subscript notation and the present context, Equation (1.26) becomes

$$P(\{\mathbf{R}|\mathbf{t_n}\})\psi^{\mathbf{k}p}_{jr}(\mathbf{r}) = \sum_{k=1}^{M(\mathbf{k})}\sum_{j=1}^{d_p} \Gamma^{\mathbf{k}p}(\{\mathbf{R}|\mathbf{t_n}\})_{kt,jr}\psi^{\mathbf{k}p}_{kt}(\mathbf{r}). \tag{7.27}$$

(a) It follows from Equations (7.23) that

$$\mathbf{\Gamma}^{\mathbf{k}p}(\{\mathbf{1}|\mathbf{t_n}\})_{kt,jr} = \delta_{jk}\delta_{tr}\exp\{-i(\mathbf{R}_j\mathbf{k}).\mathbf{t_n}\},$$

so, by Equation (7.27),

$$P(\{\mathbf{1}|\mathbf{t_n}\})\psi_{jr}^{\mathbf{k}p}(\mathbf{r}) = \exp\{-i(\mathbf{R}_j\mathbf{k}).\mathbf{t_n}\}\psi_{jr}^{\mathbf{k}p}(\mathbf{r}).$$

Comparison with Equations (7.12) shows that $\psi_{jr}^{\mathbf{k}p}(\mathbf{r})$ is a Bloch function with wave vector $\mathbf{R}_j\mathbf{k}$.

(b) If $\{\mathbf{R}|\mathbf{0}\} \in \mathcal{G}_0(\mathbf{k})$, Equations (7.23) imply that

$$\Gamma^{\mathbf{k}p}\{\mathbf{R}|\mathbf{0}\}_{kt,1r} = \delta_{k1}\,\Gamma^p_{\mathcal{G}_0(\mathbf{k})}(\{\mathbf{R}|\mathbf{0}\})_{tr}\,.$$

Then, by Equation (7.27), for $\{\mathbf{R}|\mathbf{0}\} \in \mathcal{G}_0(\mathbf{k})$

$$P(\{\mathbf{R}|\mathbf{0}\})\psi_{1r}^{\mathbf{k}p}(\mathbf{r}) = \sum_{t=1}^{d_p}\Gamma^p_{\mathcal{G}_0(\mathbf{k})}(\{\mathbf{R}|\mathbf{0}\})_{tr}\psi_{1t}^{\mathbf{k}p}(\mathbf{r}).$$

(c) From Equations (7.23)

$$\Gamma^{\mathbf{k}p}(\{\mathbf{R}_j|\mathbf{0}\})_{kt,1r} = \delta_{jk}\delta_{tr}\,,$$

so that, by Equation (7.27), $P(\{\mathbf{R}_j|\mathbf{0}\})\psi_{1r}^{\mathbf{k}p}(\mathbf{r}) = \psi_{jr}^{\mathbf{k}p}(\mathbf{r})$.

This latter theorem has a converse.

Theorem IV Suppose that $\phi_r^{\mathbf{k}p}(\mathbf{r})$, $r = 1, 2, \ldots, d_p$, are Bloch functions, with wave vector $\mathbf{k}$, that are also basis functions of the unitary irreducible representation $\mathbf{\Gamma}^p_{\mathcal{G}_0(\mathbf{k})}$ of $\mathcal{G}_0(\mathbf{k})$. Let

$$\psi_{jr}^{\mathbf{k}p}(\mathbf{r}) = P(\{\mathbf{R}_j|\mathbf{0}\})\phi_r^{\mathbf{k}p}(\mathbf{r}),\ j = 1, 2, \ldots, M(\mathbf{k}). \tag{7.28}$$

Then the set of $d_pM(\mathbf{k})$ functions $\psi_{jr}^{\mathbf{k}p}(\mathbf{r})$ forms a basis for the irreducible representation $\mathbf{\Gamma}^{\mathbf{k}p}$ of $\mathcal{G}$ defined by Equations (7.23).

Proof All that has to be shown is that the functions $\psi_{jr}^{\mathbf{k}p}(\mathbf{r})$, as defined in Equation (7.28), satisfy Equation (7.27). This follows immediately from the identity

$$P(\{\mathbf{R}|\mathbf{t_n}\})P(\{\mathbf{R}_j|\mathbf{0}\}) = P(\{\mathbf{R}_k|\mathbf{0}\})P(\{\mathbf{1}|\mathbf{R}_k^{-1}\mathbf{t_n}\})P(\{\mathbf{R}_k^{-1}\mathbf{R}\mathbf{R}_j|\mathbf{0}\}),$$

in which $\mathbf{R}_k$ can be chosen so that $\{\mathbf{R}_k^{-1}\mathbf{R}\mathbf{R}_j|\mathbf{0}\} \in \mathcal{G}_0(\mathbf{k})$.

The analysis of Chapter 6, Section 1, demonstrates that considerable simplification of the calculation of electronic energy eigenvalues can be achieved

if the energy eigenfunctions corresponding to an irreducible representation of the group of the Schrödinger equation are expanded in terms of basis functions of that representation. Moreover, it is sufficient to restrict attention just to functions transforming as one row of the irreducible representation. In the present context, the group of the Schrödinger equation is a symmorphic space group $\mathcal{G}$, and so for an energy eigenvalue corresponding to $\mathbf{\Gamma}^{\mathbf{k}p}$ it is sufficient to restrict attention to functions transforming as the $j = 1$, $r = 1$ row of $\mathbf{\Gamma}^{\mathbf{k}p}$, that is, to Bloch functions with wave vector $\mathbf{k}$ that transform under the rotations of $\mathcal{G}_0(\mathbf{k})$ as the first row of $\mathbf{\Gamma}^p_{\mathcal{G}_0(\mathbf{k})}$.

Such "symmetrized wave functions" can be constructed using the projection operator technique described in Chapter 5, Section 1. Applied to spherical harmonics, plane waves or atomic orbitals this technique produces the "symmetrized spherical harmonics", "symmetrized plane waves" or "symmetrized atomic orbitals" that are needed for the various methods of electronic energy band calculation. (Good accounts of these methods exist in the reviews of Callaway (1958,1964), Fletcher (1971), Pincherle (1960,1971) and Reitz (1955).) Details of these applications of the projection operator technique may be found elsewhere (e.g. Cornwell (1969)). Tabulations of the symmetrized spherical harmonics for the space groups O_h^1, O_h^5 and O_h^9, the so-called "kubic harmonics", have been given by von der Lage and Bethe (1947), Howarth and Jones (1952), Bell (1954), Altmann (1957) and Altmann and Cracknell (1965). The construction of symmetrized plane waves for all 73 symmorphic space groups may be simplified by the use of tables given by Luehrmann (1968), which supplement those given previously for O_h^1, O_h^9 and T_d^2 by Schlosser (1962).

(b) Irreducible representations of the cubic space groups O_h^1, O_h^5 and O_h^9

The simple cubic space group O_h^1, the face-centred cubic space group O_h^5 and the body-centred cubic space group O_h^9 provide examples of symmorphic space groups of great importance. The following description of them will serve to introduce the standard notations and conventions that are used for all symmorphic space groups.

As shown by Theorem II of subsection (a), an irreducible representation of the space group $\mathcal{G}$ is specified by an allowed $\mathbf{k}$-vector and a label p of the irreducible representation of $\mathcal{G}_0(\mathbf{k})$ to which it corresponds. The convention is that the symmetry points and axes of the Brillouin zone are denoted by capital letters, as for example in Figures 7.7, 7.8 and 7.9. The irreducible representations of the corresponding point groups $\mathcal{G}_0(\mathbf{k})$ are then labelled by assigning a subscript or set of subscripts to the appropriate capital letter.

For example, the centre of the Brillouin zone for the space groups O_h^1, O_h^5 and O_h^9 is the point Γ, so that the ten irreducible representations of the point group $\mathcal{G}_0(\mathbf{k})$ for Γ (which is actually O_h) are called Γ_1, Γ_2, Γ_{12}, Γ_{15}, Γ_{25}, $\Gamma_{1'}$,$\Gamma_{2'}$, $\Gamma_{12'}$, $\Gamma_{15'}$ and $\Gamma_{25'}$ in the most commonly used notation of Bouckaert *et al.* (1936). (This assignment of subscripts is almost entirely arbitrary and

Point	Coordinates	$\mathcal{G}_0(\mathbf{k})$
Γ	$(0,0,0)$	O_h
M	$(\pi/a)(0,1,1)$	D_{4h}
R	$(\pi/a)(1,1,1)$	O_h
X	$(\pi/a)(0,0,1)$	D_{4h}
Axis	**Coordinates, $0 < \kappa < 1$**	$\mathcal{G}_0(\mathbf{k})$
Δ	$(\pi/a)(0,0,\kappa)$	C_{4v}
Λ	$(\pi/a)(\kappa,\kappa,\kappa)$	C_{3v}
Σ	$(\pi/a)(0,\kappa,\kappa)$	C_{2v}
S	$(\pi/a)(\kappa,\kappa,1)$	C_{2v}
T	$(\pi/a)(\kappa,1,1)$	C_{4v}
Z	$(\pi/a)(0,\kappa,1)$	C_{2v}
Plane	**Equation**	$\mathcal{G}_0(\mathbf{k})$
ΓMX	$k_x = 0$	$C_s(IC_{2x})$
ΓRM	$k_y = k_z > k_x$	$C_s(IC_{2f})$
ΓRX	$k_x = k_y < k_z$	$C_s(IC_{2b})$
MRX	$k_z = \pi/a$	$C_s(IC_{2z})$

Table 7.2: The point groups $\mathcal{G}_0(\mathbf{k})$ for the symmetry points, axes and planes of the simple cubic space group O_h^1

unfortunately conveys no direct information about the nature of the corresponding irreducible representation. More informative notations have been proposed by Howarth and Jones (1952) and by Bell (1954), but the notation of Bouckaert *et al.* (1936) is so widely used that to employ any other notation now would just cause confusion.)

The point groups $\mathcal{G}_0(\mathbf{k})$ for the symmetry points, axes and planes of the space groups O_h^1, O_h^5 and O_h^9 are given in Tables 7.2, 7.3 and 7.4 respectively. The notation for the point groups is that of Schönfliess (1923). This notation is used again in Appendix C, where the character tables for all 32 crystallographic point groups are listed, together with explicit sets of matrices for all irreducible representations of dimension greater than one. The tables of Appendix C also give, when appropriate, the notation of Bouckaert *et al.* (1936) for the irreducible representations of $\mathcal{G}_0(\mathbf{k})$. (The rotations of each $\mathcal{G}_0(\mathbf{k})$ listed in Appendix C are for the value of $\mathbf{k}$ specified in Tables 7.2, 7.3 and 7.4.)

It is possible for two or more points in different stars to have point groups $\mathcal{G}_0(\mathbf{k})$ that are isomorphic. In such a situation the actual group elements of the $\mathcal{G}_0(\mathbf{k})$ may be different, the isomorphic groups merely differing in the orientation of their defining axes. For example, for the body-centred cubic space group O_h^9, the points on the axes Σ and D correspond to a $\mathcal{G}_0(\mathbf{k})$ that is

Point	Coordinates	$\mathcal{G}_0(\mathbf{k})$
Γ	$(0,0,0)$	O_h
L	$(\pi/a)(1,1,1)$	D_{3d}
W	$(\pi/a)(0,1,2)$	D_{2d}
X	$(\pi/a)(0,0,2)$	D_{4h}

Axis	Coordinates	$\mathcal{G}_0(\mathbf{k})$
Δ	$(\pi/a)(0,0,2\kappa),\ 0<\kappa<1$	C_{4v}
Λ	$(\pi/a)(\kappa,\kappa,\kappa),\ 0<\kappa<1$	C_{3v}
Σ	$(\pi/a)(0,\frac{3}{2}\kappa,\frac{3}{2}\kappa),\ 0<\kappa\leq 1$	C_{2v}
Q	$(\pi/a)(1-\kappa,1,1+\kappa),\ 0<\kappa<1$	C_2
S	$(\pi/a)(\frac{1}{2}\kappa,\frac{1}{2}\kappa,2),\ 0<\kappa\leq 1$	C_{2v}
Z	$(\pi/a)(0,\kappa,2),\ 0<\kappa<1$	C_{2v}

Plane	Equation	$\mathcal{G}_0(\mathbf{k})$
ΓKWX	$k_x=0$	$C_s(IC_{2x})$
ΓKL	$k_y=k_z>k_x$	$C_s(IC_{2f})$
ΓLUX	$k_x=k_y<k_z$	$C_s(IC_{2b})$
UWX	$k_z=2\pi/a$	$C_s(IC_{2z})$

Table 7.3: The point groups $\mathcal{G}_0(\mathbf{k})$ for the symmetry points, axes and planes of the face-centred cubic space group O_h^5

C_{2v}. However, with the coordinates of Σ and D given in Table 7.4, the group elements of $\mathcal{G}_0(\mathbf{k})$ for Σ (arranged in classes) are

$$\mathcal{C}_1 = E,\ \mathcal{C}_2 = C_{2e},\ \mathcal{C}_3 = IC_{2x},\ \mathcal{C}_4 = IC_{2f},$$

whereas the group elements of $\mathcal{G}_0(\mathbf{k})$ for D are

$$\mathcal{C}_1 = E,\ \mathcal{C}_2 = C_{2x},\ \mathcal{C}_3 = IC_{2e},\ \mathcal{C}_4 = IC_{2f}.$$

The irreducible representations of $\mathcal{G}_0(\mathbf{k})$ for Σ are denoted by Σ_1, Σ_2, Σ_3 and Σ_4, while those for D are denoted by D_1, D_2, D_3 and D_4. The different sets of group elements occurring in this way are all listed in the description of the corresponding point group in Appendix C.

For every point $\mathbf{k}$ on a symmetry plane, the group $\mathcal{G}_0(\mathbf{k})$ is C_s, which contains just the identity transformation and a reflection. The appropriate reflection for each plane is indicated in parentheses in the third column of Tables 7.2, 7.3 and 7.4. The irreducible representation of C_s for which the character of the reflection is $+1$ is described as being "even" and is denoted by a $+$, and the other irreducible representation is described as being "odd" and is denoted by a $-$.

Figures 7.10 and 7.11 are examples of energy bands employing the notation described above.

Point	Coordinates	$\mathcal{G}_0(\mathbf{k})$
Γ	$(0,0,0)$	O_h
H	$(\pi/a)(0,0,2)$	O_h
N	$(\pi/a)(0,1,1)$	D_{2h}
P	$(\pi/a)(1,1,1)$	T_d
Axis	**Coordinates, $0 < \kappa < 1$**	$\mathcal{G}_0(\mathbf{k})$
Δ	$(\pi/a)(0,0,2\kappa)$	C_{4v}
Λ	$(\pi/a)(\kappa,\kappa,\kappa)$	C_{3v}
Σ	$(\pi/a)(0,\kappa,\kappa)$	C_{2v}
D	$(\pi/a)(\kappa,\kappa,1)$	C_{2v}
F	$(\pi/a)(1-\kappa,1-\kappa,1+\kappa)$	C_{3v}
G	$(\pi/a)(0,1-\kappa,1+\kappa)$	C_{2v}
Plane	**Equation**	$\mathcal{G}_0(\mathbf{k})$
ΓHN	$k_x = 0$	$C_s(IC_{2x})$
ΓNP	$k_y = k_z > k_x$	$C_s(IC_{2f})$
ΓHP	$k_x = k_y < k_z$	$C_s(IC_{2b})$
HNP	$k_y + k_z = 2\pi/a$	$C_s(IC_{2e})$

Table 7.4: The point groups $\mathcal{G}_0(\mathbf{k})$ for the symmetry points, axes and planes of the body-centred cubic space group O_h^9

8 Consequences of the fundamental theorems

(a) Degeneracies of eigenvalues and the symmetry of $\epsilon(\mathbf{k})$

Suppose first that $\mathbf{k}$ is a *general point* of the Brillouin zone. Then $\mathcal{G}_0(\mathbf{k})$ consists only of the identity transformation $\{\mathbf{1}|\mathbf{0}\}$ and so has only one irreducible representation, namely the one-dimensional representation for which $\mathbf{\Gamma}^1(\{\mathbf{1}|\mathbf{0}\}) = [1]$. As $g_0(\mathbf{k}) = 1$, it follows from Equation (7.22) that $M(\mathbf{k}) = g_0$. There is therefore only one irreducible representation of $\mathcal{G}$ corresponding to this $\mathbf{k}$, and its dimension is $M(\mathbf{k})d_1 = g_0.1 = g_0$, so that the corresponding energy eigenvalue is g_0-fold degenerate.

Any Bloch function $\exp(i\mathbf{k}.\mathbf{r})u_\mathbf{k}(\mathbf{r})$ with this wave vector $\mathbf{k}$ is a basis function for the irreducible representation of this $\mathcal{G}_0(\mathbf{k})$ and the set of basis functions of the corresponding irreducible representation of $\mathcal{G}$ formed from this function are $\exp(i\mathbf{k}.\mathbf{r})u_\mathbf{k}(\mathbf{r}), \exp(i\mathbf{k}_2.\mathbf{r})u_\mathbf{k}(\mathbf{R}_2^{-1}\mathbf{r}), \ldots$. Now suppose that these Bloch functions are energy eigenfunctions. As they correspond to wave vectors $\mathbf{k}(=\mathbf{k}_1), \mathbf{k}_2, \ldots$, they correspond, according to Equation (7.14), to energy eigenvalues $\epsilon(\mathbf{k}), \epsilon(\mathbf{k}_2), \ldots$. As they are degenerate, being a basis for an irreducible representation of $\mathcal{G}$, it follows that

$$\epsilon(\mathbf{R}_j\mathbf{k}) \equiv \epsilon(\mathbf{k}_j) = \epsilon(\mathbf{k}) \tag{7.29}$$

for $j = 1, 2, \ldots, g_0$, the $\mathbf{R}_j$ being the set of rotations of $\mathcal{G}_0$. Thus the g_0 wave

vectors in the star of $\mathbf{k}$ have the same energies, and $\epsilon(\mathbf{k})$ has the symmetry of the point group $\mathcal{G}_0$ of the space group $\mathcal{G}$. This means that if the band structure is known in one basic section of the Brillouin zone containing only $(1/g_0)$ of the volume of the Brillouin zone and no two wave vectors in the same star, then it can be obtained immediately throughout the *whole* Brillouin zone. For example, for the body-centred cubic space group O_h^9, whose Brillouin zone is shown in Figure 7.8, $g_0 = 48$ and the basic section is the wedge-shaped region ΓHNP (or, more precisely, the region bounded by the planes containing three of the four points Γ, H, N and P).

The symmetry of $\epsilon(\mathbf{k})$ is widely employed in calculations of energy band structures and in determinations of the Fermi surface from experimental measurements, such as those of the de Haas-van Alphen effect. For a general point of the Brillouin zone the inclusion of the rotational parts of $\mathcal{G}$ in addition to the translational parts of $\mathcal{T}$ already taken into account in Bloch's Theorem is of *no* assistance in simplifying the numerical task of actually finding the energy eigenvalues by the technique described in Chapter 6, Section 1. For this reason, relatively few accurate calculations of $\epsilon(\mathbf{k})$ have been performed for general points of the Brillouin zone.

The second case that will be considered is at the other extreme. For the point $\mathbf{k} = \mathbf{0}$, $\mathbf{Rk} = \mathbf{0}$ for every $\{\mathbf{R}|\mathbf{0}\}$ of $\mathcal{G}_0(\mathbf{k})$, so that $\mathcal{G}_0(\mathbf{0}) = \mathcal{G}_0$. The star of $\mathbf{k}$ then consists only of $\mathbf{k} = \mathbf{0}$ itself and so $M(\mathbf{0}) = 1$. The basis functions of $\mathcal{G}$ corresponding to $\mathbf{k} = \mathbf{0}$ are merely the periodic basis functions of $\mathcal{G}_0$, and the corresponding degeneracies of energy eigenvalues are those of the dimensions of the irreducible representations of $\mathcal{G}_0$. In this case the technique of Chapter 6, Section 1, allows an appreciable simplification of the numerical work involved in finding the energy eigenvalues, even beyond that already brought about by the consideration of $\mathcal{T}$ alone.

Some space groups possess other symmetry points for which $\mathcal{G}_0(\mathbf{k}) = \mathcal{G}_0$. These do not require further examination, as the comments made about the point $\mathbf{k} = \mathbf{0}$ also apply to these points. The point H of the Brillouin zone of the body-centred cubic lattice is an example.

The third and final case is that of the intermediate situation in which $\mathcal{G}_0(\mathbf{k})$ is not trivial but is a proper subgroup of $\mathcal{G}_0$. Included in this case are all symmetry points other than those of the second case and all points on symmetry axes and planes. For such a point $\mathcal{G}_0(\mathbf{k})$ will have more than one irreducible representation, some of these possibly being of more than one dimension. As $g_0(\mathbf{k}) < g_0$, it follows from Equation (7.22) that $M(\mathbf{k}) > 1$.

Consider the energy eigenvalue corresponding to a d_p-dimensional irreducible representation of $\mathcal{G}_0(\mathbf{k})$. This will be $d_p M(\mathbf{k})$-fold degenerate by the theorem, and this degeneracy is made up as follows:

(a) By a similar argument to that used in the case of a general point, it follows that

$$\epsilon(\mathbf{k}_j) = \epsilon(\mathbf{k}), \; j = 1, 2, \ldots, M(\mathbf{k}),$$

so that again $\epsilon(\mathbf{k})$ exhibits the symmetry of the point group $\mathcal{G}_0$.

(b) In addition, each $\epsilon(\mathbf{k}_j)$ is "d_p-fold degenerate", in the sense that there are d_p linearly independent Bloch eigenfunctions of $H(\mathbf{r})$ corresponding to this eigenvalue *and* to this particular wave vector $\mathbf{k}_j$. The degree of simplification of numerical work depends on the order $g_0(\mathbf{k})$.

These arguments show that, although the concept of a star appears in the fundamental theorems for symmorphic space groups, it is in some contexts possible and convenient to revert to the description that appeared in Section 4 with Bloch's Theorem, in which there corresponds a set of energy levels to every allowed $\mathbf{k}$-vector of the Brillouin zone and not merely to those lying in different stars. In this description, a d_p-fold degeneracy of $\epsilon(\mathbf{k})$ means, as above, that there are d_p linearly independent Bloch eigenfunctions of $H(\mathbf{r})$ corresponding to this eigenvalue and to the particular wave vector $\mathbf{k}$. A d_p-fold degeneracy of $\epsilon(\mathbf{k})$ then corresponds to a d_p-dimensional irreducible representation of $\mathcal{G}_0(\mathbf{k})$. This degeneracy was indicated in Figures 7.10 and 7.11 by $[d_p]$. Furthermore each energy band then has the symmetry of $\mathcal{G}_0$. This is the description that is commonly used in the solid state literature.

It is worth while pointing out here that even if $\mathcal{G}_0$ does not contain the spatial inversion operator I, the symmetry $\epsilon(\mathbf{k}) = \epsilon(-\mathbf{k})$ always remains because of time-reversal symmetry. (For details, see, for example, Chapter 8, Section 5, of Cornwell (1984)).

(b) Continuity and compatibility of the irreducible representations of $\mathcal{G}_0(\mathbf{k})$

A typical section of an energy band diagram for a symmetry axis is shown in Figure 7.12. The axis displayed there is the Δ axis of the cubic space groups O_h^1, O_h^5 and O_h^9. The numbers in parentheses are the band labels, as defined in Expression (7.19), so that the bands 1 and 2 "touch" at one point $\mathbf{k}_0$. This figure exhibits two general characteristics of energy bands.

The first feature is that, along any part of a band which does not touch another band, the corresponding irreducible representation of $\mathcal{G}_0(\mathbf{k})$ remains the same. Thus, for example, the whole of the left-hand part of band 1 corresponds to Δ_2 and the whole of the right-hand part to $\Delta_{1'}$. It is therefore possible to talk of *the* symmetry of a band, or part of a band, along an axis. The reason for this behaviour is essentially that the energy eigenvalues corresponding to a particular irreducible representation of $\mathcal{G}_0(\mathbf{k})$ can be obtained from a secular equation involving only basis functions of that representation, as was noted in Chapter 6, Section 1. A small change in $\mathbf{k}$ will then only produce a small change in the energy eigenvalues emerging from this secular equation.

The second general characteristic is that the symmetries of the bands are interchanged at a point where the bands touch. For example, in Figure 7.12 band 1 changes from Δ_2 to $\Delta_{1'}$ on moving from left to right, while band 2 changes from $\Delta_{1'}$ to Δ_2. The reason for this is that the secular equation corresponding to an irreducible representation of $\mathcal{G}_0(\mathbf{k})$ produces energy eigenvalues that are analytic functions of $\mathbf{k}$, the degeneracy corresponding to the

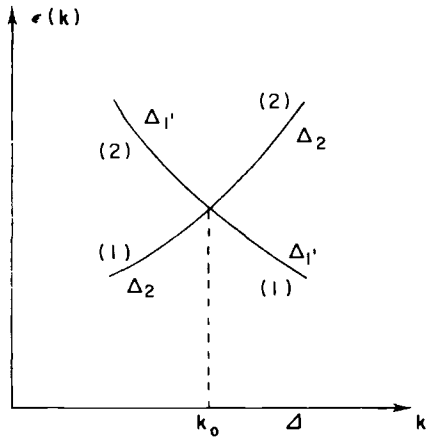

Figure 7.12: "Touching" of energy bands along the Δ axis of the cubic space groups.

touching of two bands having no effect on this as it is "accidental". This also implies that $\text{grad}_{\mathbf{k}}\epsilon(\mathbf{k})$ is continuous for bands, or parts of bands, belonging to the same irreducible representation, and this continuity is not affected by the interchange of band labels when bands touch. Thus, for example, in Figure 7.12 the limit as $\mathbf{k} \to \mathbf{k}_0$ from the left of $\text{grad}_{\mathbf{k}}\epsilon(\mathbf{k})$ for band 1 is equal to the limit as $\mathbf{k} \to \mathbf{k}_0$ from the right of $\text{grad}_{\mathbf{k}}\epsilon(\mathbf{k})$ for band 2. The "touching" of energy bands has been investigated in detail by Herring (1937).

The concept of "compatibility" is best described by an example. Consider therefore a Γ_{12} energy level at the point Γ of the Brillouin zone for the body-centred cubic space group O_h^9. This level, being two-fold degenerate, belongs to two energy bands. What then are the symmetries of these bands near Γ along the symmetry axis Δ? That is, what irreducible representations of the group $\mathcal{G}_0(\mathbf{k})$ for Δ are "compatible" with Γ_{12}?

The investigation proceeds as follows. Let $\mathcal{G}_0(\Gamma)$ and $\mathcal{G}_0(\Delta)$ be the point groups $\mathcal{G}_0(\mathbf{k})$ for $\mathbf{k}$ at Γ and on Δ respectively. Then $\mathcal{G}_0(\Delta)$ is a subgroup of $\mathcal{G}_0(\Gamma)$ and so the irreducible representations of $\mathcal{G}_0(\Gamma)$ are representations of $\mathcal{G}_0(\Delta)$ that are, in general, reducible. The actual reduction can be determined immediately from the characters, for if $\mathbf{\Gamma}$ and $\mathbf{\Gamma}^p$ are irreducible representations of $\mathcal{G}_0(\Gamma)$ and $\mathcal{G}_0(\Delta)$ respectively, with characters denoted by χ and χ^p, then the number of times n_p that $\mathbf{\Gamma}^p$ appears in the reduction of $\mathbf{\Gamma}$ is given by

$$n_p = (1/g_0(\Delta)) \sum_{\{\mathbf{R}|\mathbf{0}\}\in\mathcal{G}_0(\Delta)} \chi(\{\mathbf{R}|\mathbf{0}\})\, \chi^p(\{\mathbf{R}|\mathbf{0}\})^*,$$

where $g_0(\Delta)$ is the order of $\mathcal{G}_0(\Delta)$. (This is just an immediate application of Theorem V of Chapter 4, Section 6.) Thus, for example, the reduction of Γ_{12}

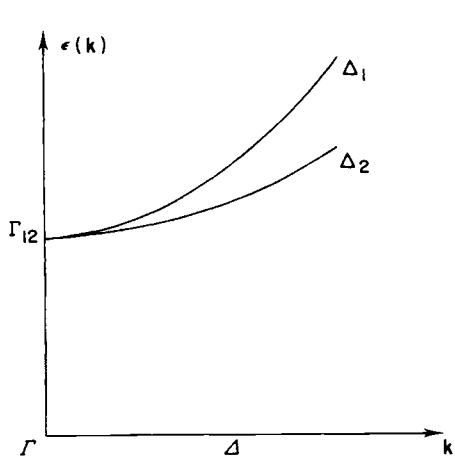

Figure 7.13: "Compatibility" of the Γ_{12} energy level with the Δ_1 and Δ_2 energy levels along the Δ axis.

in this context is given by

$$\Gamma_{12} = \Delta_1 \oplus \Delta_2.$$

The point Γ could be considered as an ordinary point of Δ by ignoring the elements of $\mathcal{G}_0(\Gamma)$ that are not in $\mathcal{G}_0(\Delta)$, and then the energy levels at Γ could be classified in terms of the irreducible representations of $\mathcal{G}_0(\Delta)$. The Γ_{12} level would then be regarded as a non-degenerate Δ_1 level and a non-degenerate Δ_2 level that happen to have the same value. Because of the continuity of irreducible representations along axes that was mentioned above, the two bands that touch at Γ in the Γ_{12} level will along the Δ axis near Γ have symmetries Δ_1 and Δ_2. The degeneracy that exists at Γ is split on moving away from Γ. This situation is shown in Figure 7.13.

Although this argument shows that the Δ_1 and Δ_2 irreducible representations are compatible with the Γ_{12} level, it cannot predict whether the band having Δ_1 symmetry lies lower or higher than the band having Δ_2 symmetry. This can only be determined by direct calculation.

The same analysis can be applied to all irreducible representations at every symmetry point for all the symmetry axes going through that point. A similar analysis can also be used to determine the compatibility of the irreducible representations corresponding to a symmetry axis with those of the symmetry planes containing the axis. These results can be expressed in "compatibility tables". A typical example is exhibited in Table 7.5. A comprehensive set of such tables for the space groups O_h^1, O_h^5 and O_h^9 was given by Bouckaert *et al.* (1936) (see also Cornwell (1969)).

It is possible to develop this type of analysis to investigate certain finer features of the electronic energy bands, particularly the vanishing of components of $\text{grad}_{\mathbf{k}}\epsilon(\mathbf{k})$ and the form of the intersection of constant energy contours with symmetry axes. This allows the location of the "critical points" (van Hove

Γ_1	Γ_2	Γ_{12}	Γ_{15}	Γ_{25}
Δ_1	Δ_2	$\Delta_1\Delta_2$	$\Delta_1\Delta_5$	$\Delta_2\Delta_5$
Σ_1	Σ_4	$\Sigma_1\Sigma_4$	$\Sigma_1\Sigma_3\Sigma_4$	$\Sigma_2\Sigma_3\Sigma_4$
Λ_1	Λ_2	Λ_3	$\Lambda_1\Lambda_3$	$\Lambda_2\Lambda_3$

$\Gamma_{1'}$	$\Gamma_{2'}$	$\Gamma_{12'}$	$\Gamma_{15'}$	$\Gamma_{25'}$
$\Delta_{1'}$	$\Delta_{2'}$	$\Delta_{1'}\Delta_{2'}$	$\Delta_{1'}\Delta_5$	$\Delta_{2'}\Delta_5$
Σ_2	Σ_3	$\Sigma_2\Sigma_3$	$\Sigma_2\Sigma_3\Sigma_4$	$\Sigma_1\Sigma_2\Sigma_3$
Λ_2	Λ_1	Λ_3	$\Lambda_2\Lambda_3$	$\Lambda_1\Lambda_3$

Table 7.5: Compatibility relations between the symmetry point Γ and the symmetry axes Δ, Σ and Λ for the cubic space groups O_h^1, O_h^5 and O_h^9.

1953, Phillips 1956) to be located. For details see Cornwell (1969), and also Rashba (1959), Sheka (1960) and Kudryavtseva (1967).

(c) Origin and orientation dependence of the symmetry labelling of electronic states

Consider, as an example, the NaCl structure, in which the Na nuclei occupy the lattice sites of one Γ_c^f lattice and the Cl nuclei occupy the lattice sites of another Γ_c^f lattice, one lattice being obtained from the other by a pure translation through $\mathbf{t}_0 = \frac{1}{2}a(1,0,0)$. (Here a is the quantity appearing in the definition of the basic lattice vectors of Γ_c^f in Table 7.1). With the origin of the coordinate system taken at one of the Na nuclei, Equation (1.13) is satisfied for every coordinate transformation T of the space group O_h^5. Similarly, with the origin at a Cl nucleus, Equation (1.13) is again satisfied for every T of O_h^5. Let $H(\mathbf{r})$ and $H'(\mathbf{r})$ be the Hamiltonian operators corresponding to these two choices of origin. Although $H(\mathbf{r})$ and $H'(\mathbf{r})$ are related, they are obviously not identical, that is, $H(\mathbf{r}) \neq H'(\mathbf{r})$.

It can be shown (Cornwell 1971) in a situation such as this that, while the actual *values* of the electronic energy levels are naturally independent of the choice of origin of the coordinate system, the *labelling* of the states in terms of the irreducible representations of the space group can be origin dependent.

The symmetry labels of states also depend on the choice of the *orientation* of the coordinate axes, as has been discussed in detail by Cornwell (1972).

Chapter 8

The Role of Lie Algebras

1 "Local" and "global" aspects of Lie groups

It is now time to begin the systematic study of Lie groups. They were introduced at an early stage in Chapter 3 so that the general features of their representation theory could be presented at the same time as the representation theory of finite groups. Although the definition of a linear Lie group given in Section 1 of Chapter 3 necessarily involved the "local" coordinates $(x_1, x_2, \ldots, x_n)$ which parametrize elements near the identity, the emphasis in the subsequent sections of that chapter was on the "global" properties (that is, the properties of the *whole* group), particularly the concept of compactness and integration on the group.

In the closer study of Lie groups both the "local" and the "global" aspects are important, but it is fair to say that most of the information concerning the structure of a Lie group comes from the investigation of its "local" properties. It is the main purpose of this chapter to show how these "local" properties are themselves determined by the corresponding "real Lie algebra". The link is provided for linear Lie groups by the matrix exponential function, which is described in Section 2, and which leads in turn to the idea of a "one-parameter subgroup" of Section 3. The concept of a real Lie algebra is introduced first for the group of proper rotations in $\mathbb{R}^3$, for which the argument (in Section 4) is helped by the geometrical nature of the elements under consideration. At the same time the very useful and closely related notion of a "complex Lie algebra" is defined. For general linear Lie groups a slightly different line of argument is needed, and this is provided in Section 5.

Chapter 9 will be mainly concerned with introducing for Lie algebras many of the ideas previously discussed for groups, and relating these to the analogous properties of linear Lie groups. Again the emphasis will be largely on the "local" aspects of the groups.

Chapter 10 is devoted to the rotation groups in $\mathbb{R}^3$, to the related groups SO(3), O(3) and SU(2), and to their Lie algebras. Not only are they important for their applications in atomic and nuclear physics, but their representations

lie at the heart of much of the representation theory that follows in later chapters.

With Chapter 11 attention begins to be concentrated on the so-called "simple" and "semi-simple" Lie algebras, which have very important physical applications, and the structure theory of the semi-simple complex Lie algebras is investigated in detail. The representation theory of semi-simple Lie algebras is described in Chapter 12.

It may be helpful to anticipate some of the discussion by alerting the reader to the fact that, although to every Lie group there is a real Lie algebra which is *unique* (up to isomorphism), in general several *non*-isomorphic Lie groups can correspond to the same real Lie algebra. Also, although to every real Lie algebra the complexification is *unique* (up to isomorphism), in general several *non*-isomorphic real Lie algebras correspond to the same complex Lie algebra.

In all the arguments that follow involving matrices, the "commutator" $[\mathbf{A}, \mathbf{B}]$ of any two $m \times m$ matrices $\mathbf{A}$ and $\mathbf{B}$ is defined by

$$[\mathbf{A}, \mathbf{B}] = \mathbf{AB} - \mathbf{BA}.$$

2 The matrix exponential function

The matrix exponential function provides the link between a linear Lie group and its corresponding real Lie algebra. Its definition and certain of its properties are simple generalizations of those of the familiar exponential function of a real or complex number.

Definition *The matrix exponential function*
If $\mathbf{a}$ is an $m \times m$ matrix, then $\exp \mathbf{a}$ is the $m \times m$ matrix defined by

$$\exp \mathbf{a} = \mathbf{1} + \sum_{j=1}^{\infty} \mathbf{a}^j / j! \,. \tag{8.1}$$

Theorem I The series for $\exp \mathbf{a}$ in Equation (8.1) converges for *any* $m \times m$ matrix $\mathbf{a}$.

Proof See, for example, Chapter 10, Section 2, of Cornwell (1984).

The following example will prove to be very significant.

Example I *The proper rotation matrices* $\mathbf{R}(T)$ *of* SO(3) *as matrix exponential functions*
Consider the 3×3 matrix $\mathbf{a}_1$ defined by

$$\mathbf{a}_1 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}. \tag{8.2}$$

Then, with $\mathbf{a} = \theta \mathbf{a}_1$, $\mathbf{a}^j = (-1)^{(j-1)/2}\theta^j \mathbf{a}_1$ for j *odd*, and

$$\mathbf{a}^j = (-1)^{j/2}\theta^j \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

for j *even*, so that

$$\exp(\theta \mathbf{a}_1) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{bmatrix}. \tag{8.3}$$

As noted in Chapter 1, Section 1, the right-hand side of Equation (8.3) specifies a proper rotation through an angle θ in the right-hand screw sense about the axis Ox (cf. Equation (1.3)). It will be demonstrated in Section 4 that *every* matrix of SO(3) can be expressed in matrix exponential form with a suitable choice of exponent.

The multiplication properties of matrix exponential functions are more complicated than those of exponential functions of real or complex numbers, as the following theorem shows.

Theorem II

(a) If $\mathbf{a}$ and $\mathbf{b}$ are any $m \times m$ matrices that *commute*,

$$(\exp \mathbf{a})(\exp \mathbf{b}) = \exp(\mathbf{a} + \mathbf{b}) = (\exp \mathbf{b})(\exp \mathbf{a}). \tag{8.4}$$

(b) If $\mathbf{a}$ and $\mathbf{b}$ are $m \times m$ matrices whose entries are sufficiently small

$$(\exp \mathbf{a})(\exp \mathbf{b}) = \exp \mathbf{c},$$

where

$$\mathbf{c} = \mathbf{a} + \mathbf{b} + \frac{1}{2}[\mathbf{a}, \mathbf{b}] + \frac{1}{12}\{[\mathbf{a}, [\mathbf{a}, \mathbf{b}]] + [\mathbf{b}, [\mathbf{b}, \mathbf{a}]]\} + \ldots, \tag{8.5}$$

where the infinite series in Equation (8.5) contains commutators of increasingly higher order. Thus, in general,

$$(\exp \mathbf{a})(\exp \mathbf{b}) \neq (\exp \mathbf{b})(\exp \mathbf{a}).$$

Equation (8.5) is known as the "Campbell-Baker-Hausdorff formula".

Proof

(a) If $[\mathbf{a}, \mathbf{b}] = \mathbf{0}$ then $(\mathbf{a} + \mathbf{b})^j = \sum_{k=0}^{j} \{j!/(k!(j-k)!)\}\mathbf{a}^k \mathbf{b}^{j-k}$, so that Equations (8.4) follow in exactly the same way as the corresponding results for real or complex numbers.

(b) The precise conditions on the smallness of the elements of $\mathbf{a}$ and $\mathbf{b}$ required to ensure the convergence of the series in Equation (8.5), together with the complete expression for $\mathbf{c}$, may be found in the original papers (Campbell 1897a,b, Baker 1905, Hausdorff 1906). All that will be done here is to demonstrate the correctness of Equation (8.5) to second order. From Equation (8.1) (to second order)

$$\begin{aligned}(\exp\mathbf{a})(\exp\mathbf{b}) &= \{\mathbf{1}+\mathbf{a}+\frac{1}{2}\mathbf{a}^2+\ldots\}\{\mathbf{1}+\mathbf{b}+\frac{1}{2}\mathbf{b}^2+\ldots\} \\ &= \mathbf{1}+(\mathbf{a}+\mathbf{b})+(\frac{1}{2}\mathbf{a}^2+\mathbf{ab}+\frac{1}{2}\mathbf{b}^2)+\ldots \qquad (8.6)\end{aligned}$$

However, to second order,

$$\begin{aligned}\exp\mathbf{c} &= \exp\{\mathbf{a}+\mathbf{b}+\frac{1}{2}[\mathbf{a},\mathbf{b}]+\ldots\} \\ &= \mathbf{1}+\{(\mathbf{a}+\mathbf{b})+\frac{1}{2}[\mathbf{a},\mathbf{b}]+\ldots\} \\ &\quad +\frac{1}{2}\{(\mathbf{a}+\mathbf{b})+\frac{1}{2}[\mathbf{a},\mathbf{b}]+\ldots\}^2+\ldots \\ &= \mathbf{1}+\{\mathbf{a}+\mathbf{b}+\frac{1}{2}(\mathbf{ab}-\mathbf{ba})+\ldots\} \\ &\quad +\frac{1}{2}\{\mathbf{a}^2+\mathbf{ba}+\mathbf{ab}+\mathbf{b}^2+\ldots\}+\ldots, \qquad (8.7)\end{aligned}$$

from which Equation (8.5) follows to second order, on equating the right-hand sides of Equations (8.6) and (8.7).

Theorem III The matrix exponential function formed from an $m \times m$ matrix $\mathbf{a}$ possesses the following properties:

(a) $(\exp\mathbf{a})^\star = \exp(\mathbf{a}^\star)$.

(b) The transpose of $(\exp\mathbf{a})$ is $\exp(\tilde{\mathbf{a}})$.

(c) $(\exp\mathbf{a})^\dagger = \exp(\mathbf{a}^\dagger)$.

(d) For any $m \times m$ non-singular matrix $\mathbf{S}$

$$\exp(\mathbf{SaS}^{-1}) = \mathbf{S}(\exp\mathbf{a})\mathbf{S}^{-1}.$$

(e) If $\lambda_1, \lambda_2, \ldots, \lambda_m$ are the eigenvalues of $\mathbf{a}$, then $e^{\lambda_1}, e^{\lambda_2}, \ldots, e^{\lambda_m}$ are the eigenvalues of $\exp\mathbf{a}$.

(f) $\det(\exp\mathbf{a}) = \exp(\mathrm{tr}\,\mathbf{a})$.

(g) $\exp\mathbf{a}$ is always non-singular and

$$(\exp\mathbf{a})^{-1} = \exp(-\mathbf{a}).$$

(h) The mapping $\phi(\mathbf{a}) = \exp \mathbf{a}$ is a one-to-one continuous mapping of a small neighbourhood of the $m \times m$ zero matrix $\mathbf{0}$ onto a small neighbourhood of the $m \times m$ unit matrix $\mathbf{1}$.

Proof See, for example, Appendix E, Section 1, of Cornwell (1984).

3 One-parameter subgroups

Definition *One-parameter subgroup of a linear Lie group*
A "one-parameter subgroup" of a linear Lie group $\mathcal{G}$ is a Lie subgroup of $\mathcal{G}$ consisting of elements $T(t)$ which depend on a real parameter t that takes all values from $-\infty$ to $+\infty$ such that

$$T(s)T(t) = T(s+t) \tag{8.8}$$

for all s and t, $-\infty < s, t < +\infty$.

In particular, if $\mathcal{G}$ is a group of $m \times m$ matrices then a one-parameter subgroup of $\mathcal{G}$ is a Lie subgroup of matrices $\mathbf{A}(t)$ such that

$$\mathbf{A}(s)\mathbf{A}(t) = \mathbf{A}(s+t) \tag{8.9}$$

for all s and t, $-\infty < s, t < +\infty$.

Clearly $T(s)T(t) = T(t)T(s)$ for all s and t, so every one-parameter subgroup is Abelian. Moreover, Equation (8.8) with $s = 0$ implies that $T(0) = E$, the identity of $\mathcal{G}$. Obviously a one-parameter subgroup is a Lie group of dimension 1, so that in the matrix case $d\mathbf{A}/dt$ for $t = 0$ exists and is not identically zero.

Example I *A one-parameter subgroup of* SO(3)
The 3×3 matrices $\mathbf{A}(t)$ defined by

$$\mathbf{A}(t) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos t & \sin t \\ 0 & -\sin t & \cos t \end{bmatrix}$$

satisfy Equation (8.9) and form a subgroup of SO(3) that is (by Equation (3.7)) isomorphic to the Lie group SO(2). Thus these matrices form a one-parameter subgroup of SO(3). As shown by Example I of Section 2, $\mathbf{A}(t) = \exp(t\mathbf{a}_1)$, where $\mathbf{a}_1$ is specified by Equation (8.2).

The property exhibited in this example is completely general, as the following theorem shows.

Theorem I Every one-parameter subgroup of a linear Lie group $\mathcal{G}$ of $m \times m$ matrices is formed by exponentiation of $m \times m$ matrices. Indeed, if the

matrices $\mathbf{A}(t)$ form a one-parameter subgroup of $\mathcal{G}$, then

$$\mathbf{A}(t) = \exp\{t\mathbf{a}\}, \tag{8.10}$$

where $\mathbf{a} = d\mathbf{A}/dt$ evaluated at $t = 0$.

Proof For brevity write $\dot{\mathbf{A}}(t) = d\mathbf{A}/dt$, so $\mathbf{a} = \dot{\mathbf{A}}(0)$. Let

$$\mathbf{B}(t) = \mathbf{A}(t)\exp\{-t\dot{\mathbf{A}}(0)\},$$

so that $\dot{\mathbf{B}}(t) = \{\dot{\mathbf{A}}(t) - \mathbf{A}(t)\dot{\mathbf{A}}(0)\}\exp\{-t\dot{\mathbf{A}}(0)\}$. However, from Equation (8.9), for any t,

$$\dot{\mathbf{A}}(t) = \lim_{s\to 0}[\mathbf{A}(t+s) - \mathbf{A}(t)]/s = \lim_{s\to 0}\mathbf{A}(t)[\mathbf{A}(s) - \mathbf{A}(0)]/s,$$

so that

$$\dot{\mathbf{A}}(t) = \mathbf{A}(t)\dot{\mathbf{A}}(0). \tag{8.11}$$

Thus $\dot{\mathbf{B}}(t) = 0$ for all t and consequently $\mathbf{B}(t) = \mathbf{B}(0) = \mathbf{1}$, from which Equation (8.10) follows immediately.

4 Lie algebras

For the linear Lie group SO(3) it will now be shown that it is possible to introduce the corresponding real Lie algebra in a very direct way by a combination of algebraic and geometric arguments. For the other linear Lie groups the essential results are similar, but the arguments are rather longer and less direct.

It is essential to bear in mind that, in this context, there are *three* mutually isomorphic groups, namely

(a) the groups of all proper rotations T in $\mathbb{R}^3$,

(b) the group SO(3) of rotation matrices $\mathbf{R}(T)$, and

(c) the corresponding group of linear operators $P(T)$ (as defined in Equation (1.17)).

Consider first *any* proper rotation T in $\mathbb{R}^3$. Suppose this is a rotation through an angle θ_0 about a certain axis. Then the set of *all* rotations about that axis form a one-parameter subgroup. Consequently *every proper rotation lies in some one-parameter subgroup of the group of proper rotations in* $\mathbb{R}^3$. Correspondingly, every matrix of SO(3) must lie in some one-parameter subgroup of SO(3). By the theorem of Section 3, if $\mathbf{A}(t)$ are the elements of such a one-parameter subgroup of SO(3), there exists a non-zero 3×3 matrix $\mathbf{a}$ such that $\mathbf{A}(t) = \exp(t\mathbf{a})$. As $\mathbf{A}(t)$ is real, Theorem III of Section 2 implies that $\mathbf{a}$ also can be taken to be real. This theorem and the condition $\widetilde{\mathbf{A}}(t) = \mathbf{A}(t)^{-1}$ also imply that $\widetilde{\mathbf{a}} = -\mathbf{a}$. Conversely, if $\mathbf{a}$ is real and $\widetilde{\mathbf{a}} = -\mathbf{a}$,

then $\mathbf{A}(t) = \exp(t\mathbf{a})$ is a member of SO(3). Thus *every element of* SO(3) *is obtained by exponentiation from some* 3×3 *real antisymmetric matrix.*

The set of all 3×3 real antisymmetric matrices forms a three-dimensional real vector space (see Appendix B, Section 1). (It forms a real vector space because, if $\mathbf{a}$ and $\mathbf{b}$ are any two such matrices, then so too is $\alpha\mathbf{a} + \beta\mathbf{b}$, for any real numbers α and β. The dimension is three because, for any such matrix $\mathbf{a}$, $a_{11} = a_{22} = a_{33} = 0$ and $a_{21} = -a_{12}$, $a_{31} = -a_{13}$, and $a_{23} = -a_{32}$.) Consequently $\mathbf{a}$ can be specified by three real parameters, such as its a_{12}, a_{13} and a_{23} elements. A convenient basis for this vector space is formed by the matrices

$$\mathbf{a}_1 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}, \quad \mathbf{a}_2 = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad \mathbf{a}_3 = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{8.12}$$

These generate one-parameter subgroups of matrices $\mathbf{R}(T)$ corresponding to rotations about Ox, Oy and Oz respectively (cf. the Examples of Sections 2 and 3).

As the commutator $[\mathbf{a}, \mathbf{b}]$ $(= \mathbf{ab} - \mathbf{ba})$ of two real 3×3 antisymmetric matrices is also a real 3×3 antisymmetric matrix, $[\mathbf{a}, \mathbf{b}]$ is a member of the vector space whenever $\mathbf{a}$ and $\mathbf{b}$ are members. Thus the set of all 3×3 real antisymmetric matrices satisfy the conditions in the following definition of a "real Lie algebra".

Definition *Real Lie algebra* $\mathcal{L}$

A "real Lie algebra" $\mathcal{L}$ of dimension n (≥ 1) is a real vector space of dimension n equipped with a "Lie product" or "commutator" $[a, b]$ defined for every a and b of $\mathcal{L}$ such that

(i) $[a, b] \in \mathcal{L}$ for all $a, b \in \mathcal{L}$;

(ii) for all $a, b, c \in \mathcal{L}$ and all real numbers α and β

$$[\alpha a + \beta b, c] = \alpha[a, c] + \beta[b, c]; \tag{8.13}$$

(iii) $[a, b] = -[b, a]$ for all $a, b \in \mathcal{L}$; and

(iv) for all $a, b, c \in \mathcal{L}$

$$[a, [b, c]] + [b, [c, a]] + [c, [a, b]] = 0. \tag{8.14}$$

(This is known as "Jacobi's identity".)

In the particular case of a Lie algebra of *matrices* the commutator $[\mathbf{a}, \mathbf{b}]$ will always be *defined* by

$$[\mathbf{a}, \mathbf{b}] = \mathbf{ab} - \mathbf{ba}, \tag{8.15}$$

and then conditions (ii), (iii) and (iv) are automatically satisfied. Similarly, for a Lie algebra of *linear operators* the commutator $[a, b]$ will always be *defined* by

$$[a, b]\phi = a(b\phi) - b(a\phi). \tag{8.16}$$

for any pair of linear operators a and b and for any element ϕ of the vector space in which they act for which the right-hand side of Equation (8.16) is meaningful.

It is not absolutely essential to have an explicit definition of $[a, b]$ in terms of other possibly simpler products such as those of Equation (8.15) or (8.16). Indeed, it is an interesting intellectual exercise to proceed solely on the basis of the properties (i), (ii), (iii) and (iv) without making any other assumptions about the nature of $[a, b]$. The resulting development is the theory of "abstract" Lie algebras. This does not lead to any new structures, for there exists a theorem by Ado (1947) which states that *every* abstract Lie algebra is isomorphic to a Lie algebra of matrices with the commutator defined as in Equation (8.15). Nevertheless, much of the development of abstract Lie algebras is no more complicated than the corresponding theory for matrices, and indeed has the additional advantage that it applies equally to matrices and linear operators as special cases. Consequently the formulation will be given in general terms whenever it is convenient to do so.

This is certainly the case for certain immediate consequences of the definition. For example, (ii) and (iii) imply that

$$[a, \beta b + \gamma c] = \beta[a, b] + \gamma[a, c] \tag{8.17}$$

for all $a, b, c \in \mathcal{L}$ and all real numbers β and γ. Further, let $a_1, a_2, \ldots, a_n$ be a basis of the real vector space of $\mathcal{L}$. As $[a_p, a_q] \in \mathcal{L}$ for all $p, q = 1, 2, \ldots, n$, there exists a set of n^3 real numbers c^r_{pq} known as the "*structure constants* of $\mathcal{L}$ with respect to the basis $a_1, a_2, \ldots, a_n$", that are defined by

$$[a_p, a_q] = \sum_{r=1}^{n} c^r_{pq} a_r, \quad p, q = 1, 2, \ldots, n. \tag{8.18}$$

(Conditions (iii) and (iv) of the definition of $\mathcal{L}$ imply that $c^r_{pq} = -c^r_{qp}$ (for $p, q = 1, 2, \ldots, n$), and $\sum_{s=1}^{n}\{c^s_{pq}c^t_{rs} + c^s_{qr}c^t_{ps} + c^s_{rp}c^t_{qs}\} = 0$ (for $p, q, r, t = 1, 2, \ldots, n$), so these constants are not independent.) Then, if $a = \sum_{p=1}^{n} \alpha_p a_p$ and $b = \sum_{q=1}^{n} \beta_q a_q$ are *any* two elements of $\mathcal{L}$ (so that $\alpha_1, \alpha_2, \ldots, \alpha_n$ and $\beta_1, \beta_2, \ldots, \beta_n$ are all real), by Equations (8.13), (8.17) and (8.18),

$$[a, b] = \sum_{p,q,r=1}^{n} \alpha_p \beta_q c^r_{pq} a_r. \tag{8.19}$$

Thus *every commutator can be evaluated from a knowledge of the structure constants.*

In particular, in the real Lie algebra $\mathcal{L} = \mathrm{so}(3)$ associated with SO(3), with the basis elements $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$ defined by Equations (8.12),

$$[\mathbf{a}_1, \mathbf{a}_2] = -\mathbf{a}_3, \ [\mathbf{a}_2, \mathbf{a}_3] = -\mathbf{a}_1, \ [\mathbf{a}_3, \mathbf{a}_1] = -\mathbf{a}_2. \tag{8.20}$$

Consequently the structure constants with respect to $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$ are given by

$$-c^r_{pq} = \epsilon_{pqr} = \begin{cases} 1, & \text{if } (p,q,r) = (1,2,3),(2,3,1),(3,1,2), \\ -1, & \text{if } (p,q,r) = (2,1,3),(1,3,2),(3,2,1), \\ 0, & \text{for all other values of } (p,q,r). \end{cases} \tag{8.21}$$

The Campbell-Baker-Hausdorff formula (see Section 2) then indicates that the product of any two elements of the *group* SO(3) lying close to the identity can be determined (at least in principle) from the structure constants. That is, *the structure of the group* SO(3) *close to its identity is specified by the structure of its corresponding real Lie algebra* $\mathcal{L}$ (=so(3)).

The commutation relations (Equations (8.20)) take a very familiar form when the real Lie algebra associated with the group of linear operators $P(T)$ corresponding to the group of proper rotations in $\mathbb{R}^3$ is considered. Let T be the rotation corresponding to the matrix $\exp(t\mathbf{a})$ of SO(3), so that, by Equation (1.17),

$$P(T)f(\mathbf{r}) = f(\{\exp(t\mathbf{a})\}^{-1}\mathbf{r}) = f(\{\exp(-t\mathbf{a})\}\mathbf{r}).$$

As $\mathbf{a} = \lim_{t\to 0}\{\exp(t\mathbf{a}) - \mathbf{1}\}/t$, it is natural to *define* a corresponding linear operator $P(\mathbf{a})$ by the same limiting process. That is, let

$$P(\mathbf{a}) = \lim_{t\to 0}\{P(\exp(t\mathbf{a})) - P(\mathbf{1})\}/t.$$

Thus, for any function $f(\mathbf{r})$ in the domain of $P(\mathbf{a})$,

$$P(\mathbf{a})f(\mathbf{r}) = \lim_{t\to 0}[f(\{\exp(-t\mathbf{a})\}\mathbf{r}) - f(\mathbf{r})]/t.$$

However, for small t,

$$\begin{aligned} f(\{\exp(-t\mathbf{a})\}\mathbf{r}) &\simeq f(\{\mathbf{1} - t\mathbf{a} + \ldots\}\mathbf{r}) = f(\mathbf{r} - t\mathbf{a}\mathbf{r} + \ldots) \\ &\simeq f(\mathbf{r}) - t\tilde{\mathbf{r}}\tilde{\mathbf{a}}\,\mathbf{grad}\, f(\mathbf{r}), \end{aligned}$$

so that

$$P(\mathbf{a}) = -\tilde{\mathbf{r}}\tilde{\mathbf{a}}\,\mathbf{grad}. \tag{8.22}$$

(Here $\mathbf{r}$ and $\mathbf{grad}$ are to be interpreted as 3×1 column matrices with entries x, y, z and $\partial/\partial x, \partial/\partial y, \partial/\partial z$ respectively.) Thus, from Equations (8.12),

$$\left.\begin{aligned} P(\mathbf{a}_1) &= y\partial/\partial z - z\partial/\partial y, \\ P(\mathbf{a}_2) &= z\partial/\partial x - x\partial/\partial z, \\ P(\mathbf{a}_3) &= x\partial/\partial y - y\partial/\partial x. \end{aligned}\right\} \tag{8.23}$$

Equation (8.22) implies that

$$[P(\mathbf{a}), P(\mathbf{b})] = P([\mathbf{a}, \mathbf{b}]). \tag{8.24}$$

In particular, by Equations (8.20), (or directly from Equations (8.23)),

$$\left.\begin{array}{rcl} [P(\mathbf{a}_1), P(\mathbf{a}_2)] & = & -P(\mathbf{a}_3), \\ [P(\mathbf{a}_2), P(\mathbf{a}_3)] & = & -P(\mathbf{a}_1), \\ [P(\mathbf{a}_3), P(\mathbf{a}_1)] & = & -P(\mathbf{a}_2). \end{array}\right\} \tag{8.25}$$

The key observation is that the quantum mechanical orbital angular momentum operators L_x, L_y and L_z are just multiples of $P(\mathbf{a}_1)$, $P(\mathbf{a}_2)$ and $P(\mathbf{a}_3)$. In fact

$$L_x = (\hbar/i)P(\mathbf{a}_1),\ L_y = (\hbar/i)P(\mathbf{a}_2),\ L_z = (\hbar/i)P(\mathbf{a}_3), \tag{8.26}$$

(see Schiff (1968)), so that Equations (8.25) imply the familiar angular momentum commutation relations

$$[L_x, L_y] = i\hbar L_z,\ [L_y, L_z] = i\hbar L_x,\ [L_z, L_x] = i\hbar L_y. \tag{8.27}$$

There is therefore an intimate connection between the quantum theory of angular momentum and the group of proper rotations in $\mathbb{R}^3$.

In particular, it will be shown in Chapter 10, Section 4, that the determination of the basis functions of the irreducible representations of the group of proper rotations in $\mathbb{R}^3$ can be reduced to the construction of the simultaneous eigenfunctions of the orbital angular momentum operators L_z and L^2, where L^2 is defined by

$$L^2 = {L_x}^2 + {L_y}^2 + {L_z}^2.$$

This latter problem is treated in nearly every book on elementary quantum mechanics (e.g. Schiff (1968)). These eigenfunctions and their corresponding eigenvalues can be found by solving certain differential equations (see Chapter 10, Section 4), but there exists a well-known, purely *algebraic* method of determining the eigenvalues (see Chapter 10, Section 3). It will become apparent that it is merely the prototype of a method that is applicable to the representations of a large class of Lie algebras.

The details of this development will be given in Chapter 10, Section 4, but it is convenient to note here that the argument for angular momentum operators involves the "ladder operators" L_+ and L_-, defined by $L_\pm = L_x \pm iL_y$, that is, it involves the operators $P(\mathbf{a}_1) \pm iP(\mathbf{a}_2)$. The significant point is the appearance here of the imaginary number i, indicating that it is useful to extend the definition of a Lie algebra to embrace such complex linear combinations. The resulting structure is called a "*complex* Lie algebra".

Definition *Complex Lie algebra* $\mathcal{L}$

A "complex Lie algebra" $\mathcal{L}$ of dimension n (≥ 1) is a *complex* vector space of dimension n equipped with a "Lie product" or "commutator" possessing the properties (i), (ii), (iii) and (iv) listed in the definition of a real Lie algebra, except that in (ii) α and β are now any *complex* numbers.

Equations (8.17), (8.18) and (8.19) apply also to complex Lie algebras (although now the α and β of (8.17), the structure constants c_{pq}^r of (8.18), and the $\alpha_1, \alpha_2, \ldots, \alpha_n$ and $\beta_1, \beta_2, \ldots, \beta_n$ of (8.19) may be *complex* numbers).

In the case of a real Lie algebra of matrices or of linear operators whose basis elements are linearly independent over the *complex* field there is no difficulty in "complexifying" the real Lie algebra to produce a unique complex Lie algebra of the same dimension. In these situations the complex vector space may be taken to have the same basis elements as the real vector space, but, in the complex space, complex linear combinations of these basis elements are allowed. In fact this is the process already encountered in connection with the angular momentum ladder operators. (For the more general case the process is rather more elaborate. See, for example, the detailed discussion of Chapter 13, Section 3, of Cornwell (1984).)

Somewhat paradoxically, the study of complex Lie algebras is more straightforward than that of real Lie algebras. Consequently it is convenient to investigate the properties of a linear Lie group by first introducing the corresponding real Lie algebra, and then proceeding almost immediately to the associated complex Lie algebra.

This section will be concluded with a definition that applies equally to real and complex Lie algebras:

Definition *Abelian Lie algebra*
A Lie algebra $\mathcal{L}$ is said to be "Abelian" if $[a, b] = 0$ for all $a, b \in \mathcal{L}$.

Thus in an Abelian Lie algebra all the structure constants are zero. Such a Lie algebra may alternatively be called "commutative".

5 The real Lie algebras that correspond to general linear Lie groups

For $\mathcal{G} = \mathrm{SO}(3)$ it was elementary to demonstrate the occurrence of one-parameter subgroups, the existence of the corresponding real Lie algebra following from these. However, for a *general* linear Lie group $\mathcal{G}$ it is necessary to reverse the order of the argument. First (in subsection (a)) it will be shown that for every such $\mathcal{G}$ a corresponding real Lie algebra of matrices exists, and only then (in subsection (b)) will the existence and properties of the one-parameter subgroups of $\mathcal{G}$ be deduced.

(a) The existence of a real Lie algebra $\mathcal{L}$ for every linear Lie group $\mathcal{G}$

As a preliminary, the essential points of the definition of a linear Lie group $\mathcal{G}$ of dimension n given in Chapter 3, Section 1, will be re-cast in the special case in which $\mathcal{G}$ actually *consists* of $m \times m$ matrices $\mathbf{A}$ (so that $T = \mathbf{A}$ and $\mathbf{\Gamma}(T) = \mathbf{A}$). There is a one-to-one correspondence between these matrices lying close to the identity and the points in $\mathbb{R}^n$ satisfying Condition (3.2) which define the matrix function $\mathbf{A}(x_1, x_2, \ldots, x_n)$ $(\in \mathcal{G})$, for all $(x_1, x_2, \ldots, x_n)$ satisfying Condition (3.2). By assumption the elements of $\mathbf{A}(x_1, x_2, \ldots, x_n)$ are analytic

functions of $x_1, x_2, \ldots, x_n$. The n $m \times m$ matrices $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n$ defined by

$$(\mathbf{a}_p)_{jk} = (\partial A_{jk}/\partial x_p)_{x_1=x_2=\ldots=x_n=0} \tag{8.28}$$

(for $j, k = 1, 2, \ldots, m$; $p = 1, 2, \ldots, n$) (cf. Equation (3.3)) then form the basis for an n-dimensional real vector space V.

Definition *Analytic curve in $\mathcal{G}$*
Let $x_1(t), x_2(t), \ldots, x_n(t)$ be a set of real analytic functions of t defined in some interval $[0, t_0)$, where $t_0 > 0$, such that $x_j(0) = 0$ for $j = 1, 2, \ldots, n$, and the point $(x_1(t), x_2(t), \ldots, x_n(t))$ satisfies Condition (3.2) for all t in $[0, t_0)$. Then the corresponding set of $m \times m$ matrices $\mathbf{A}(t)$ of $\mathcal{G}$, defined by $\mathbf{A}(t) = \mathbf{A}(x_1(t), x_2(t), \ldots, x_n(t))$, is said to form an "analytic curve" in $\mathcal{G}$.

As $\mathbf{A}(0) = \mathbf{1}$, every analytic curve starts from the identity of $\mathcal{G}$. There is no requirement at this stage that an analytic curve must form part of a one-parameter subgroup of $\mathcal{G}$.

Definition *Tangent vector of an analytic curve in $\mathcal{G}$*
The "tangent vector" of an analytic curve $\mathbf{A}(t)$ in $\mathcal{G}$ is defined to be the $m \times m$ matrix $\mathbf{a}$, where $\mathbf{a} = d\mathbf{A}(t)/dt$ evaluated at $t = 0$. (More precisely, this is the tangent vector "at the identity", but this extra phase will be omitted as no other tangent vectors will be considered here.)

Theorem I The tangent vector of any analytic curve in $\mathcal{G}$ is a member of the real vector space V having the matrices $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n$ of Equation (8.28) as its basis. Conversely, every member of V is the tangent vector of some analytic curve in $\mathcal{G}$.

Proof As $d\mathbf{A}(t)/dt = \sum_{p=1}^{n} (\partial \mathbf{A}/\partial x_p)(dx_p/dt)$, it follows then that $\mathbf{a} = \sum_{p=1}^{n} \dot{x}_p(0)\mathbf{a}_p$, where $\dot{x}_p(0) = (dx_p/dt)_{t=0}$. Thus $\mathbf{a} \in V$.

Conversely, suppose $\mathbf{a} = \sum_{p=1}^{n} \lambda_p \mathbf{a}_p$ is any member of V. Then $x_j(t) = \lambda_j t$, $j = 1, 2, \ldots, n$, defines an analytic curve that has $\mathbf{a}$ as its tangent vector.

Theorem II If $\mathbf{a}$ and $\mathbf{b}$ are the tangent vectors of the analytic curves $\mathbf{A}(t)$ and $\mathbf{B}(t)$ in $\mathcal{G}$, then $[\mathbf{a}, \mathbf{b}]$ $(= \mathbf{ab} - \mathbf{ba})$ is the tangent vector of the analytic curve $\mathbf{C}(t)$ in $\mathcal{G}$, where

$$\mathbf{C}(t) = \mathbf{A}(\sqrt{t})\mathbf{B}(\sqrt{t})\mathbf{A}(\sqrt{t})^{-1}\mathbf{B}(\sqrt{t})^{-1}. \tag{8.29}$$

Proof Theorem II of Chapter 3, Section 1, implies that the curve $\mathbf{C}(t)$ defined by Equation (8.29) is an *analytic* curve in $\mathcal{G}$. With $s = \sqrt{t}$, $\mathbf{A}(s) = \mathbf{1} + s\mathbf{a} + \frac{1}{2}s^2\mathbf{a}' + \ldots$ and $\mathbf{B}(s) = \mathbf{1} + s\mathbf{b} + \frac{1}{2}s^2\mathbf{b}' + \ldots$, where $\mathbf{a}' = (d^2\mathbf{A}/dt^2)_{t=0}$ and $\mathbf{b}' = (d^2\mathbf{B}/dt^2)_{t=0}$. Then, to second order, $\mathbf{A}(s)^{-1} = \mathbf{1} - s\mathbf{a} + s^2(\mathbf{a}^2 - \frac{1}{2}\mathbf{a}') + \ldots$ and $\mathbf{B}(s)^{-1} = \mathbf{1} - s\mathbf{b} + s^2(\mathbf{b}^2 - \frac{1}{2}\mathbf{b}') + \ldots$. Thus, after some algebra, $\mathbf{C}(t) = \mathbf{1} + s^2[\mathbf{a}, \mathbf{b}] + \ldots$, so that $(d\mathbf{C}/dt)_{t=0} = [\mathbf{a}, \mathbf{b}]$.

This leads immediately to the fundamental theorem:

Theorem III *For every linear Lie group $\mathcal{G}$ there exists a corresponding real Lie algebra $\mathcal{L}$ of the same dimension.* More precisely, if $\mathcal{G}$ has dimension n then the $m \times m$ matrices $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n$ defined by Equation (8.28) form a basis for $\mathcal{L}$.

Proof All that has to be shown is that if $\mathbf{a}$ and $\mathbf{b}$ are any two members of V, the real vector space with basis $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n$ of Equation (8.28), then so is $[\mathbf{a}, \mathbf{b}]$. However, by Theorem I above, $\mathbf{a}$ and $\mathbf{b}$ are tangent vectors to some analytic curves $\mathbf{A}(t)$ and $\mathbf{B}(t)$ in $\mathcal{G}$. Then, by Theorem II, $[\mathbf{a}, \mathbf{b}]$ is the tangent vector of the analytic curve $\mathbf{C}(t)$ of Equation (8.29), so $[\mathbf{a}, \mathbf{b}]$ must be a member of V.

Having shown that the vector space V with basis $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n$ is actually a real Lie algebra, henceforth V will be denoted by $\mathcal{L}$ (as in the statement of Theorem III above).

In the mathematical physics literature $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n$ are often referred to as the "generators" of the Lie algebra $\mathcal{L}$. While the above construction of $\mathcal{L}$ depends explicitly on the parametrization of $\mathcal{G}$, it can be shown that a different parametrization merely produces a Lie algebra that is isomorphic to $\mathcal{L}$ (in the sense of Chapter 9, Section 3). That is, the real Lie algebra corresponding to a linear Lie group is essentially unique. This will become very clear in many cases of interest after the role of the one-parameter subgroups is developed in subsection (b).

Henceforth the convention will be adopted that for the linear Lie groups SU(N), U(N), SO(N) and so on, the corresponding real Lie algebras are denoted by su(N), u(N), so(N) and so on.

Example I *The real Lie algebra $\mathcal{L} = \mathrm{su}(2)$ of the linear Lie group $\mathcal{G} = \mathrm{SU}(2)$.* It follows from Example III of Chapter 3, Section 1, and from Equation (8.28) that the generators of $\mathcal{L} = \mathrm{su}(2)$ are

$$\mathbf{a}_1 = \frac{1}{2}\begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix}, \quad \mathbf{a}_2 = \frac{1}{2}\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad \mathbf{a}_1 = \frac{1}{2}\begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}, \tag{8.30}$$

so that, by direct calculation, the basic commutation relations are

$$[\mathbf{a}_1, \mathbf{a}_2] = -\mathbf{a}_3, \quad [\mathbf{a}_2, \mathbf{a}_3] = -\mathbf{a}_1, \quad [\mathbf{a}_3, \mathbf{a}_1] = -\mathbf{a}_2. \tag{8.31}$$

It will be observed that $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$ are all traceless anti-Hermitian matrices, so $\mathcal{L}$ is the set of *all* 2×2 traceless anti-Hermitian matrices. (This result will be derived more directly in Example II below.)

This example also demonstrates that the *matrices* of a *real* Lie algebra *need not* themselves be *real*, for clearly $\mathbf{a}_1$ and $\mathbf{a}_3$ are not real. The reality condition of a real Lie algebra $\mathcal{L}$ requires *only* that the elements of $\mathcal{L}$ be *real linear combinations* of $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n$.

Theorem III has the following converse:

Theorem IV *Every* real Lie algebra is isomorphic to the real Lie algebra of some linear Lie group.

Proof See Freudenthal and de Vries (1969).

(b) The relationship of the real Lie algebra $\mathcal{L}$ to the one-parameter subgroups of $\mathcal{G}$

Theorem V Every element $\mathbf{a}$ of the real Lie algebra $\mathcal{L}$ of a linear Lie group $\mathcal{G}$ is associated with a one-parameter subgroup of $\mathcal{G}$ defined by

$$\mathbf{A}(t) = \exp(t\mathbf{a})$$

for $-\infty < t < \infty$.

Proof See, for example, Appendix E, Section 2, of Cornwell (1984).

Clearly all elements of $\mathcal{L}$ of the form $\lambda\mathbf{a}$, where λ ranges over all real values but $\mathbf{a}$ is fixed, give the *same* one-parameter subgroup of $\mathcal{G}$.

Theorem VI *Every* element of a linear Lie group $\mathcal{G}$ in some *small neighbourhood* of its identity belongs to some one-parameter subgroup of $\mathcal{G}$. That is, every such element of $\mathcal{G}$ can be obtained by exponentiating some element of the corresponding real Lie algebra.

Proof For any set of n real numbers $(x'_1, x'_2, \ldots, x'_n)$, define the $m \times m$ matrix $\mathbf{A}(x'_1, x'_2, \ldots, x'_n)$ by

$$\mathbf{A}(x'_1, x'_2, \ldots, x'_n) = \exp\{x'_1\mathbf{a}_1 + x'_2\mathbf{a}_2 + \ldots + x'_n\mathbf{a}_n\}, \tag{8.32}$$

$\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n$ being the basis of $\mathcal{L}$. That $\mathbf{A}(x'_1, x'_2, \ldots, x'_n) \in \mathcal{G}$ is guaranteed by Theorem V. Consequently the original parameters $x_1, x_2, \ldots, x_n$ can be expressed as analytic functions of $x'_1, x'_2, \ldots, x'_n$, with $x_1 = x_2 = \ldots = x_n = 0$ corresponding to $x'_1 = x'_2 = \ldots = x'_n = 0$. As the Jacobian (dx_j/dx'_k) is non-zero at $x_1 = x_2 = \ldots = x_n = 0$, this is a one-to-one mapping between small neighbourhoods of the two origins. It follows that *every* element of $\mathcal{G}$ in some small neighbourhood can be expressed in the form of Equation (8.32).

It is worth noting that as the set of coordinates $(x'_1, x'_2, \ldots, x'_n)$ of Equation (8.32) satisfies all the conditions of Chapter 3, Section 1, it provides an alternative to the original set $x_1, x_2, \ldots, x_n$, and because it is necessarily simply related to $\mathcal{L}$ it is called a set of "canonical coordinates" for $\mathcal{G}$.

There remains the question of whether this result extends to the *whole* of the connected subgroup of $\mathcal{G}$. The next theorem shows that this is so if $\mathcal{G}$ is

compact, but it is possible to construct examples that demonstrate that this need *not* be so if $\mathcal{G}$ is *non-compact*. (See, for example, Example III of Chapter 10, Section 5, of Cornwell (1984)).

Theorem VII If $\mathcal{G}$ is a *compact* linear Lie group, *every* element of the connected subgroup of $\mathcal{G}$ can be expressed in the form $\exp \mathbf{a}$ for some element $\mathbf{a}$ of the corresponding real Lie algebra $\mathcal{L}$. In particular, if $\mathcal{G}$ is connected and compact, every element of $\mathcal{G}$ has the form $\exp \mathbf{a}$ for some $\mathbf{a} \in \mathcal{L}$.

Proof See Price (1977) or Dynkin and Oniscik (1955).

Even for compact connected Lie groups this mapping need not be one-to-one, for it is possible that $\exp \mathbf{a} = \exp \mathbf{b}$ with $\mathbf{a} \neq \mathbf{b}$. For example, for $\mathcal{G} = \mathrm{SO}(3)$ Equation (8.3) shows that $\exp(\theta \mathbf{a}_1) = \exp\{(\theta + 2\pi n)\mathbf{a}_1\}$ for $n = \pm 1, \pm 2, \ldots$.

The exponential mapping provides a direct way of determining the real Lie algebras corresponding to a number of important linear Lie groups that does not require an explicit parametrization. The following example illustrates the method.

Example II *The real Lie algebra* $\mathcal{L} = \mathrm{su}(N)$ *for* $\mathcal{G} = \mathrm{SU}(N)$ *for* $N \geq 2$. Let $\exp(t\mathbf{a})$ be any one-parameter subgroup of $\mathcal{G} = \mathrm{SU}(N)$, so that $\mathbf{a}$ is some $N \times N$ matrix. As $\exp(t\mathbf{a})$ is required to be unitary, parts (c) and (g) of Theorem III of Section 2 imply that

$$\mathbf{a}^\dagger = -\mathbf{a}. \tag{8.33}$$

Moreover, as it is required that $\det(\exp(t\mathbf{a})) = 1$ for all real t, part (f) of that theorem shows that $\exp(\mathrm{tr}\,(t\mathbf{a})) = 1$ for all real t. Clearly this is only possible if

$$\mathrm{tr}\,\mathbf{a} = 0. \tag{8.34}$$

Thus $\mathcal{L} = \mathrm{su}(N)$ *is the set of all traceless anti-Hermitian* $N \times N$ *matrices.*

The dimension n of $\mathcal{L}$ (and hence of $\mathcal{G}$) can be calculated as follows. Equation (8.33) implies that the diagonal elements of $\mathbf{a}$ must all be purely imaginary. Taking Equation (8.34) into account, the set of diagonal elements is specified by $N - 1$ real parameters. (For example, $ia_{11}, ia_{22}, \ldots, ia_{N-1,N-1}$ may be taken to have arbitrary real values, but $a_{NN} = -\sum_{j=1}^{N-1} a_{jj}$.) Similarly, Equation (8.33) implies that the "lower" off-diagonal elements of $\mathbf{a}$ (i.e. the a_{jk} with $j > k$) are completely specified by the corresponding "upper" off-diagonal elements, as $a_{kj} = -a_{jk}{}^\star$. There are $\frac{1}{2}(N^2 - N)$ upper off-diagonal elements, and as each has an independent real and imaginary part, the set of all off-diagonal elements is specified by $2.\frac{1}{2}(N^2 - N)(= (N^2 - N)$ real parameters. Thus $\mathbf{a}$ $(\in \mathcal{L})$ requires $(N^2 - N) + (N - 1)(= (N^2 - 1))$ real parameters, or, put another way, there exist $N^2 - 1$ linearly independent traceless anti-Hermitian $N \times N$ matrices. Hence $n = N^2 - 1$.

In particular, $n = 3$ for $\mathcal{G} = \mathrm{SU}(2)$, and $n = 8$ for $\mathcal{G} = \mathrm{SU}(3)$.

$\mathcal{G}$	Conditions on $\mathbf{A} \in \mathcal{G}$	$\mathcal{L}$	Conditions on $\mathbf{a} \in \mathcal{L}$	n
$\mathrm{GL}(N,\mathbb{C})$	-	$\mathrm{gl}(N,\mathbb{C})$	-	$2N^2$
$\mathrm{GL}(N,\mathbb{R})$	$\mathbf{A}$ real	$\mathrm{gl}(N,\mathbb{R})$	$\mathbf{a}$ real	N^2
$\mathrm{SL}(N,\mathbb{C})$	$\det \mathbf{A} = 1$	$\mathrm{sl}(N,\mathbb{C})$	$\mathrm{tr}\,\mathbf{a} = 0$	$2N^2 - 2$
$\mathrm{SL}(N,\mathbb{R})$	$\begin{cases} \mathbf{A} \text{ real}, \\ \det \mathbf{A} = 1 \end{cases}$	$\mathrm{sl}(N,\mathbb{R})$	$\begin{cases} \mathbf{a} \text{ real}, \\ \mathrm{tr}\,\mathbf{a} = 0 \end{cases}$	$N^2 - 1$
$\mathrm{U}(N)$	$\mathbf{A}^\dagger = \mathbf{A}^{-1}$	$\mathrm{u}(N)$	$\mathbf{a}^\dagger = -\mathbf{a}$	N^2
$\mathrm{SU}(N)$	$\begin{cases} \mathbf{A}^\dagger = \mathbf{A}^{-1}, \\ \det \mathbf{A} = 1 \end{cases}$	$\mathrm{su}(N)$	$\begin{cases} \mathbf{a}^\dagger = -\mathbf{a}, \\ \mathrm{tr}\,\mathbf{a} = 0 \end{cases}$	$N^2 - 1$
$\mathrm{U}(p,q)$	$\mathbf{A}^\dagger \mathbf{g} = \mathbf{g}\mathbf{A}^{-1}$	$\mathrm{u}(p,q)$	$\mathbf{a}^\dagger \mathbf{g} = -\mathbf{g}\mathbf{a}$	N^2
$\mathrm{SU}(p,q)$	$\begin{cases} \mathbf{A}^\dagger \mathbf{g} = \mathbf{g}\mathbf{A}^{-1}, \\ \det \mathbf{A} = 1 \end{cases}$	$\mathrm{su}(p,q)$	$\begin{cases} \mathbf{a}^\dagger \mathbf{g} = -\mathbf{g}\mathbf{a}, \\ \mathrm{tr}\,\mathbf{a} = 0 \end{cases}$	$N^2 - 1$
$\mathrm{O}(N,\mathbb{C})$	$\tilde{\mathbf{A}} = \mathbf{A}^{-1}$	$\mathrm{so}(N,\mathbb{C})$	$\tilde{\mathbf{a}} = -\mathbf{a}$	$N^2 - N$
$\mathrm{SO}(N,\mathbb{C})$	$\begin{cases} \tilde{\mathbf{A}} = \mathbf{A}^{-1}, \\ \det \mathbf{A} = 1 \end{cases}$	$\mathrm{so}(N,\mathbb{C})$	$\tilde{\mathbf{a}} = -\mathbf{a}$	$N^2 - N$
$\mathrm{O}(N)$	$\begin{cases} \tilde{\mathbf{A}} = \mathbf{A}^{-1}, \\ \mathbf{A} \text{ real} \end{cases}$	$\mathrm{so}(N)$	$\begin{cases} \tilde{\mathbf{a}} = -\mathbf{a}, \\ \mathbf{a} \text{ real} \end{cases}$	$\frac{1}{2}(N^2 - N)$
$\mathrm{SO}(N)$	$\begin{cases} \tilde{\mathbf{A}} = \mathbf{A}^{-1}, \\ \mathbf{A} \text{ real}, \\ \det \mathbf{A} = 1 \end{cases}$	$\mathrm{so}(N)$	$\begin{cases} \tilde{\mathbf{a}} = -\mathbf{a}, \\ \mathbf{a} \text{ real} \end{cases}$	$\frac{1}{2}(N^2 - N)$
$\mathrm{O}(p,q)$	$\begin{cases} \tilde{\mathbf{A}}\mathbf{g} = \mathbf{g}\mathbf{A}^{-1}, \\ \mathbf{A} \text{ real} \end{cases}$	$\mathrm{so}(p,q)$	$\begin{cases} \tilde{\mathbf{a}}\mathbf{g} = -\mathbf{g}\mathbf{a}, \\ \mathbf{a} \text{ real} \end{cases}$	$\frac{1}{2}(N^2 - N)$
$\mathrm{SO}(p,q)$	$\begin{cases} \tilde{\mathbf{A}}\mathbf{g} = \mathbf{g}\mathbf{A}, \\ \mathbf{A}^{-1} \text{ real}, \\ \det \mathbf{A} = 1 \end{cases}$	$\mathrm{so}(p,q)$	$\begin{cases} \tilde{\mathbf{a}}\mathbf{g} = -\mathbf{g}\mathbf{a}, \\ \mathbf{a} \text{ real} \end{cases}$	$\frac{1}{2}(N^2 - N)$
$\mathrm{SO}^*(N)$	$\begin{cases} \tilde{\mathbf{A}} = \mathbf{A}^{-1}, \\ \mathbf{A}^\dagger \mathbf{J}\mathbf{A} = \mathbf{J} \end{cases}$	$\mathrm{so}^*(N)$	$\begin{cases} \tilde{\mathbf{a}} = -\mathbf{a}, \\ \mathbf{a}^\dagger \mathbf{J} = -\mathbf{J}\mathbf{a} \end{cases}$	$\frac{1}{2}(N^2 - N)$
$\mathrm{Sp}(\frac{N}{2},\mathbb{C})$	$\tilde{\mathbf{A}}\mathbf{J}\mathbf{A} = \mathbf{J}$	$\mathrm{sp}(\frac{N}{2},\mathbb{C})$	$\tilde{\mathbf{a}}\mathbf{J} = -\mathbf{J}\mathbf{a}$	$N^2 + N$
$\mathrm{Sp}(\frac{N}{2},\mathbb{R})$	$\begin{cases} \tilde{\mathbf{A}}\mathbf{J}\mathbf{A} = \mathbf{J}, \\ \mathbf{A} \text{ real} \end{cases}$	$\mathrm{sp}(\frac{N}{2},\mathbb{R})$	$\begin{cases} \tilde{\mathbf{a}}\mathbf{J} = -\mathbf{J}\mathbf{a}, \\ \mathbf{a} \text{ real} \end{cases}$	$\frac{1}{2}(N^2 + N)$
$\mathrm{Sp}(\frac{N}{2})$	$\begin{cases} \tilde{\mathbf{A}}\mathbf{J}\mathbf{A} = \mathbf{J}, \\ \mathbf{A}^\dagger = \mathbf{A}^{-1} \end{cases}$	$\mathrm{sp}(\frac{N}{2})$	$\begin{cases} \tilde{\mathbf{a}}\mathbf{J} = -\mathbf{J}\mathbf{a}, \\ \mathbf{a}^\dagger = -\mathbf{a} \end{cases}$	$\frac{1}{2}(N^2 + N)$
$\mathrm{Sp}(r,s)$	$\begin{cases} \tilde{\mathbf{A}}\mathbf{J}\mathbf{A} = \mathbf{J}, \\ \mathbf{A}^\dagger \mathbf{G}\mathbf{A} = \mathbf{G} \end{cases}$	$\mathrm{sp}(r,s)$	$\begin{cases} \tilde{\mathbf{a}}\mathbf{J} = -\mathbf{J}\mathbf{a}, \\ \mathbf{a}^\dagger \mathbf{G} = -\mathbf{G}\mathbf{a} \end{cases}$	$\frac{1}{2}(N^2 + N)$
$\mathrm{SU}^*(N)$	$\begin{cases} \mathbf{J}\mathbf{A}^\star = \mathbf{A}\mathbf{J}, \\ \det \mathbf{A} = 1 \end{cases}$	$\mathrm{su}^*(N)$	$\begin{cases} \mathbf{J}\mathbf{a}^\star = \mathbf{a}\mathbf{J}, \\ \mathrm{tr}\,\mathbf{a} = 0 \end{cases}$	$N^2 - 1$

Table 8.1: The real Lie algebras $\mathcal{L}$ of some important linear Lie groups $\mathcal{G}$. $\mathbf{A}$ and $\mathbf{a}$ are $N \times N$ matrices, which are complex unless otherwise stated; $\mathbf{g}$ is an $N \times N$ diagonal matrix with p diagonal elements $+1$ and q $(= N - p)$ diagonal elements -1, $p \geq q \geq 1$. In the last six entries N is even, and $\mathbf{J}$ and $\mathbf{G}$ are the $N \times N$ matrices defined in Equations (8.35) and (8.36).

Table 8.1 lists the details of the real Lie algebras belonging to a number of important linear Lie groups that can be obtained this way. In Table 8.1 $\mathbf{J}$ and $\mathbf{G}$ are the $N \times N$ matrices defined by

$$\mathbf{J} = \begin{bmatrix} \mathbf{0} & \mathbf{1}_{N/2} \\ -\mathbf{1}_{N/2} & \mathbf{0} \end{bmatrix}, \tag{8.35}$$

and

$$\mathbf{G} = \begin{bmatrix} -\mathbf{1}_r & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{1}_s & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & -\mathbf{1}_r & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{1}_s \end{bmatrix}, \tag{8.36}$$

where $1 \leq r \leq \frac{1}{2}N$ and $s = \frac{1}{2}N - r$.

That the exponential mapping remains invaluable even for *non-compact* linear Lie groups is demonstrated by the following theorem.

Theorem VIII *Every* element of the connected subgroup of *any* linear Lie group $\mathcal{G}$ can be expressed as a *finite* product of exponentials of its real Lie algebra $\mathcal{L}$.

Proof See, for example, Appendix E, Section 2, of Cornwell (1984).

These results may be *summarized* by the statement that the matrix exponential function *always* provides a mapping of $\mathcal{L}$ *into* $\mathcal{G}$. This is *onto* if $\mathcal{G}$ connected and *compact*, and even when $\mathcal{G}$ is connected but *non-compact* every element of $\mathcal{G}$ is expressible as a *finite* product of exponentials of members of $\mathcal{L}$.

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Chapter 9

The Relationships between Lie Groups and Lie Algebras Explored

1 Introduction

This chapter is concerned primarily with introducing for Lie algebras a number of concepts that were defined in previous chapters for groups, and then investigating in detail the relationships between these concepts for a linear Lie group and its corresponding real Lie algebra. For the most part these relationships are very straightforward, but in some instances there are complications in which the global aspects of the Lie groups make themselves apparent.

Section 2 introduces the idea of a subalgebra and Section 3 examines isomorphic and homomorphic mappings for Lie algebras. This enables the basic ideas of representation theory for Lie algebras to be developed in Section 4. Section 5 is devoted to the study of the so-called "adjoint" representations, which are defined for both Lie algebras and Lie groups and which play an important role in later chapters. The chapter is concluded in Section 6 with an investigation of direct sums of Lie algebras and their representations.

2 Subalgebras of Lie algebras

The definitions that follow apply equally to real or complex Lie algebras.

Definition *Subalgebra of a Lie algebra*
A "subalgebra" $\mathcal{L}'$ of a Lie algebra $\mathcal{L}$ is a subset of elements of $\mathcal{L}$ that themselves form a Lie algebra with the same commutator and field as that of $\mathcal{L}$.

This implies that $\mathcal{L}'$ is real if $\mathcal{L}$ is real and $\mathcal{L}'$ is complex if $\mathcal{L}$ is complex.

$\mathcal{L}'$ is said to be a "proper" subalgebra of $\mathcal{L}$ if at least one element of $\mathcal{L}$ is not contained in $\mathcal{L}'$. In this case the dimension of $\mathcal{L}'$ is smaller than that of $\mathcal{L}$. (Throughout this book the convention will be adopted that every Lie algebra and subalgebra has dimension *greater than zero.*)

Definition *Invariant subalgebra of a Lie algebra*
A subalgebra $\mathcal{L}'$ of a Lie algebra $\mathcal{L}$ is said to be "invariant" if $[a, b] \in \mathcal{L}'$ for all $a \in \mathcal{L}'$ and $b \in \mathcal{L}$.

An alternative name for an invariant subalgebra is an "ideal".

In the special case of a real Lie algebra of matrices the following theorems show that there is an intimate connection between these concepts and the corresponding concepts for linear Lie groups.

Theorem I If $\mathcal{G}$ and $\mathcal{G}'$ are linear Lie groups, $\mathcal{L}$ and $\mathcal{L}'$ are their corresponding real Lie algebras and $\mathcal{G}'$ is a subgroup of $\mathcal{G}$, then $\mathcal{L}'$ is a subalgebra of $\mathcal{L}$. Moreover, if $\mathcal{G}'$ is an *invariant* subgroup of $\mathcal{G}$, then $\mathcal{L}'$ is an *invariant* subalgebra of $\mathcal{L}$.

Proof See, for example, Appendix E, Section 3, of Cornwell (1984).

Theorem II Let $\mathcal{L}$ be the real Lie algebra corresponding to a linear Lie group $\mathcal{G}$. Then each subalgebra of $\mathcal{L}$ is the Lie algebra of exactly one connected Lie subgroup of $\mathcal{G}$.

Proof See Helgason (1962, 1978).

This section will be concluded with a useful result on invariant subalgebras. Let $\mathcal{L}'$ and $\mathcal{L}''$ be two subspaces of a Lie algebra $\mathcal{L}$ and let $[\mathcal{L}', \mathcal{L}'']$ denote the subset of $\mathcal{L}$ that consists of all linear combinations (with coefficients in the same field as that of $\mathcal{L}$) of elements of the form $[a', a'']$, where $a' \in \mathcal{L}'$ and $a'' \in \mathcal{L}''$.

Theorem III If $\mathcal{L}'$ and $\mathcal{L}''$ are invariant subalgebras of $\mathcal{L}$, then $[\mathcal{L}', \mathcal{L}'']$ is also an invariant subalgebra of $\mathcal{L}$ (or it is the "trivial" set consisting only of the zero element 0 of $\mathcal{L}$).

Proof See, for example, Appendix E, Section 3, of Cornwell (1984).

3 Homomorphic and isomorphic mappings of Lie algebras

The following definitions apply equally to real and complex Lie algebras, the "field" being the set of all real numbers in the first case and the set of all complex numbers in the second. The concepts are in essence the same for

Lie algebras as for groups, that is, homomorphisms are structure-preserving mappings and isomorphisms are homomorphisms that are one-to-one.

Definition *Homomorphic mapping of a Lie algebra $\mathcal{L}$ onto a Lie algebra $\mathcal{L}'$* Let ψ be a mapping of a Lie algebra $\mathcal{L}$ onto a Lie algebra $\mathcal{L}'$ having the same field such that

(i) for all $a, b \in \mathcal{L}$ and all α, β of the field

$$\psi(\alpha a + \beta b) = \alpha\psi(a) + \beta\psi(b); \tag{9.1}$$

and

(ii) for all $a, b \in \mathcal{L}$

$$\psi([a, b]) = [\psi(a), \psi(b)]. \tag{9.2}$$

Then ψ is said to be a "homomorphic" mapping of $\mathcal{L}$ onto $\mathcal{L}'$.

Definition *Isomorphic mapping of a Lie algebra $\mathcal{L}$ onto a Lie algebra $\mathcal{L}'$* A mapping ψ of a Lie algebra $\mathcal{L}$ onto a Lie algebra $\mathcal{L}'$ with the same field is said to be "isomorphic" if it is both homomorphic and one-to-one.

In the special case in which $\mathcal{L}'$ is identical to $\mathcal{L}$ (so that ψ is a mapping of $\mathcal{L}$ onto itself) an isomorphic mapping is called an "automorphism". With the product of two automorphisms ϕ and ψ of $\mathcal{L}$ defined by $(\phi\psi(a) = \phi(\psi(a))$ (for all $a \in \mathcal{L}$), the set of all automorphisms of $\mathcal{L}$ forms a *group*, which will be denoted by $\mathrm{Aut}(\mathcal{L})$.

Theorem I Suppose that there exists a homomorphic mapping ψ of a Lie algebra $\mathcal{L}$ onto a Lie algebra $\mathcal{L}'$ with the same field. Then $\mathcal{L}$ and $\mathcal{L}'$ have the same dimension if and only if ψ is an isomorphic mapping.

Proof Suppose that $a_1, a_2, \ldots, a_n$ is a basis of $\mathcal{L}$ and consider the equation $\sum_{j=1}^{n} \alpha_j \psi(a_j) = 0$, where $\alpha_1, \alpha_2, \ldots, \alpha_n$ are members of the field of $\mathcal{L}$ (and $\mathcal{L}'$). By virtue of Equation (9.1), this equation can be rewritten as $\psi(\sum_{j=1}^{n} \alpha_j a_j) = 0$. If ψ is one-to-one, this implies that $\sum_{j=1}^{n} \alpha_j a_j = 0$, which, because of the linear independence of $a_1, a_2, \ldots, a_n$, has only the solution $\alpha_1 = \alpha_2 = \ldots = \alpha_n = 0$. Consequently $\psi(a_1), \psi(a_2), \ldots, \psi(a_n)$ must also be linearly independent.

Conversely, if $\psi(a_1), \psi(a_2), \ldots, \psi(a_n)$ are linearly independent then the only solution of $\psi(a) = 0$ is $a = 0$. (This follows as any such a can be written as $a = \sum_{j=1}^{n} \alpha_j a_j$, so $\psi(a)(= \sum_{j=1}^{n} \alpha_j \psi(a_j)) = 0$ implies $\alpha_1 = \alpha_2 = \ldots = \alpha_n = 0$ and hence $a = 0$). Thus ψ is one-to-one (for if $\psi(b) = \psi(b')$, then $\psi(b - b') = 0$ and hence $b - b' = 0$, implying that $b = b'$).

In order to directly connect these notions with those for linear Lie groups, it is necessary to modify the definition of homomorphic mappings for linear Lie groups.

Definition *Analytic homomorphism of a linear Lie group $\mathcal{G}$ onto a linear Lie group $\mathcal{G}'$*
Let ϕ be a mapping of a linear Lie group $\mathcal{G}$ onto a linear Lie group $\mathcal{G}'$ such that

(i) ϕ is a homomorphic mapping in the "abstract" group sense of the definition of Chapter 2, Section 6; and, *in addition*,

(ii) for every $\mathbf{A}(x_1, x_2, \ldots, x_n) \in \mathcal{G}$ in some small neighbourhood of the identity of $\mathcal{G}$, $\phi(\mathbf{A}(x_1, x_2, \ldots, x_n))$ is a matrix whose elements are *analytic* functions of $x_1, x_2, \ldots, x_n$ (in the sense of Chapter 3, Section 1).

Then ϕ is said to be an "analytic" homomorphism of $\mathcal{G}$ onto $\mathcal{G}'$.

(Strictly speaking, the above definition requires only that ϕ be analytic at the identity of $\mathcal{G}$. However, it can be shown (Sagle and Walde 1973) that such a homomorphism is necessarily analytic on the *whole* of $\mathcal{G}$. Consequently nothing is lost in calling such a homomorphism "analytic" without further qualification.)

In a similar way it is possible to define a "*continuous* homomorphism" of a connected linear Lie group $\mathcal{G}$ onto a connected linear Lie group $\mathcal{G}'$ as a mapping that is a homomorphism in the abstract group sense and is continuous in the sense that the elements of the matrix $\phi(\mathbf{A}(y_1, y_2, \ldots, y_n))$ are *continuous* functions of the parameters $y_1, y_2, \ldots, y_n$ of the connected subgroup of $\mathcal{G}$ (see Chapter 3, Section 2). It is a very remarkable fact that if a homomorphic mapping is continuous then it is certainly analytic. (For a proof see, for example, Sagle and Walde (1973).)

Definition *Analytic isomorphism of a linear Lie group $\mathcal{G}$ onto a linear Lie group $\mathcal{G}'$*
This is simply an analytic homomorphism that is also one-to-one.

Theorem II If $\mathcal{G}$ and $\mathcal{G}'$ are two linear Lie groups and $\mathcal{L}$ and $\mathcal{L}'$ are their corresponding real Lie algebras, and if ϕ is an analytic homomorphic mapping of $\mathcal{G}$ onto $\mathcal{G}'$, then the mapping ψ of $\mathcal{L}$ into $\mathcal{L}'$ defined for each $\mathbf{a} \in \mathcal{L}$ by

$$\psi(\mathbf{a}) = \left[\tfrac{d}{dt}\{\phi(\exp(t\mathbf{a}))\}\right]_{t=0} \tag{9.3}$$

is a homomorphic mapping of $\mathcal{L}$ onto $\mathcal{L}'$. Moreover, for all $\mathbf{a} \in \mathcal{L}$ and $-\infty < t < \infty$

$$\exp\{t\psi(\mathbf{a})\} = \phi(\exp(t\mathbf{a})). \tag{9.4}$$

Proof See, for example, Appendix E, Section 4, of Cornwell (1984).

This theorem has an obvious generalization to isomorphic mappings.

Theorem III If $\mathcal{G}$ and $\mathcal{G}'$ are two linear Lie groups and $\mathcal{L}$ and $\mathcal{L}'$ are their corresponding real Lie algebras, and if ϕ is an analytic isomorphic mapping

of $\mathcal{G}$ onto $\mathcal{G}'$, then the mapping ψ of $\mathcal{L}$ onto $\mathcal{L}'$ defined by Equation (9.3) is an isomorphism.

Proof All that has to be shown is that ψ is one-to-one. Suppose that $\psi(\mathbf{a}) = \psi(\mathbf{b})$. Then, by Equation (9.4), $\phi(\exp(t\mathbf{a})) = \phi(\exp(t\mathbf{b}))$ for all real t. If ϕ is an isomorphism this implies that $\exp(t\mathbf{a}) = \exp(t\mathbf{b})$ for all real t, so that $\mathbf{a} = \mathbf{b}$.

Example I *The analytic isomorphic mapping of* U(1) *onto* SO(2) *and the associated isomorphic mapping of their real Lie algebras*
Consider the mapping ϕ of $\mathcal{G} = \mathrm{U}(1)$ onto $\mathcal{G}' = \mathrm{SO}(2)$, defined for all real x_1 by

$$\phi([\exp(ix_1)]) = \begin{bmatrix} \cos x_1 & \sin x_1 \\ -\sin x_1 & \cos x_1 \end{bmatrix}.$$

It is easily shown that this is an analytic isomorphism. With the basis of $\mathcal{L} = \mathrm{u}(1)$ taken to be the 1×1 matrix $\mathbf{a}_1 = [i]$, by Equation (9.3)

$$\psi(\mathbf{a}_1) = \left(\frac{d}{dt}\begin{bmatrix} \cos t & \sin t \\ -\sin t & \cos t \end{bmatrix}\right)_{t=0} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}. \tag{9.5}$$

As $\mathcal{L} = \mathrm{u}(1)$ and $\mathcal{L}' = \mathrm{so}(2)$ are one-dimensional Lie algebras, they are necessarily Abelian and hence they must be isomorphic.

Much more remarkable is the next theorem, for which a preliminary definition is required.

Definition *Discrete subgroup of a linear Lie group*
A subgroup $\mathcal{K}$ of a linear Lie group $\mathcal{G}$ is said to be "discrete" if either

(i) $\mathcal{K}$ is a finite group; or

(ii) $\mathcal{K}$ has a countable infinity of elements, but there exists a small neighbourhood of the identity of $\mathcal{G}$ that contains *no* element of $\mathcal{K}$ (apart from the identity of $\mathcal{G}$ itself).

Theorem IV If the kernel $\mathcal{K}$ of an analytic homomorphic mapping ϕ of a linear Lie group $\mathcal{G}$ onto a linear Lie group $\mathcal{G}'$ is *discrete*, then the corresponding mapping ψ (defined in Equation (9.3)) of the real Lie algebra $\mathcal{L}$ of $\mathcal{G}$ onto the real Lie algebra $\mathcal{L}'$ of $\mathcal{G}'$ is an *isomorphic* mapping.

Proof If $\mathcal{K}$ is discrete there exists a small sphere S centred on the identity of $\mathcal{G}$ such that the only element in S that maps under ϕ into the identity of $\mathcal{G}'$ is the identity of $\mathcal{G}$. Consequently ϕ provides a *one-to-one* mapping of S onto a small neighbourhood of the identity of $\mathcal{G}'$. Thus $\mathcal{G}$ and $\mathcal{G}'$ must have the same dimension, which implies that $\mathcal{L}$ and $\mathcal{L}'$ have the same dimension. Theorems I and II of this section combine to show then that ψ must be an isomorphic mapping.

This result is of the greatest significance, as it shows that in general the structure of a linear Lie group is **not** *completely determined by its corresponding real Lie algebra, for two (or more) linear Lie groups that are not isomorphic can have isomorphic real Lie algebras.* The terminology used to describe this situation is that the real Lie algebra does not determine the structure of its corresponding Lie groups "globally", but only "locally". (In fact it can be shown that *all* the connected linear Lie groups having isomorphic real Lie algebras can be determined (at least in principle) from the "universal covering group" of the Lie algebra. Moreover, all semi-simple connected linear Lie groups with isomorphic Lie algebras can be constructed quite easily from the "universal linear group" of the Lie algebra, this group being itself a semi-simple connected linear Lie group. For details, see, for example, Chapter 11, Section 7, of Cornwell (1984)).

The following examples demonstrate explicitly the conclusions of the above theorem. The second is particularly important in the quantum theory of angular momentum.

Example II *The analytic homomorphic mapping of the multiplicative group of positive real numbers* $\mathbb{R}_+$ *onto the group* SO(2) *and the associated isomorphic mappings of their real Lie algebras.*
Let $\mathcal{G}$ be the multiplicative group of positive real numbers $\mathbb{R}_+$ and $\mathcal{G}'$ the group SO(2). Each element of $\mathcal{G}$ can be considered as the component of a 1×1 matrix. As shown in Examples I and II of Chapter 3, Section 1, every element of $\mathcal{G}$ then has the form $[\exp x_1]$, where x_1 can take any real value, and every element of $\mathcal{G}'$ can be written in the form of Equation (3.7). It is easily verified that the mapping ϕ defined by

$$\phi([\exp x_1]) = \begin{bmatrix} \cos x_1 & \sin x_1 \\ -\sin x_1 & \cos x_1 \end{bmatrix} \tag{9.6}$$

is an analytic homomorphism of $\mathcal{G}$ onto $\mathcal{G}'$. Clearly its kernel $\mathcal{K}$ is the set $[\exp x_1]$ with $x_1 = 2\pi k$, $k = 0, \pm 1, \pm 2, \ldots$. Although countably infinite, $\mathcal{K}$ satisfies the condition of Theorem IV, for in any neighbourhood $-\epsilon < x_1 < \epsilon$ with $0 < \epsilon < 2\pi$ the only point corresponding to an element of $\mathcal{K}$ is $x_1 = 0$, which corresponds to the identity.

It is obvious in this case that $\mathcal{G}$ and $\mathcal{G}'$ are both one-dimensional, so that $\mathcal{L}$ and $\mathcal{L}'$ are also both one-dimensional and hence necessarily isomorphic. With the basis of $\mathcal{L}$ taken to be the 1×1 matrix $\mathbf{a}_1 = [1]$, by Equations (9.3) and (9.6),

$$\psi(\mathbf{a}_1) = \left(\frac{d}{dt} \begin{bmatrix} \cos t & \sin t \\ -\sin t & \cos t \end{bmatrix} \right)_{t=0} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}.$$

It should be noted that, although $\mathcal{G}$ and $\mathcal{G}'$ have isomorphic real Lie algebras, $\mathcal{G}'$ is *compact* but $\mathcal{G}$ is *non-compact* (see Examples I and II of Chapter 3, Section 3).

Example III *The analytic homomorphic mapping of* SU(2) *onto* SO(3) *and the associated isomorphic mapping of their real Lie algebras*
Let $\mathcal{G} = \mathrm{SU}(2)$ and $\mathcal{G}' = \mathrm{SO}(3)$. It was shown in Chapter 2, Section 6, that there exists a homomorphic mapping ϕ (in the abstract group sense) of SU(2) onto SO(3) defined by

$$\phi(\mathbf{u})_{jk} = (1/2)\mathrm{tr}\{\boldsymbol{\sigma}_j \mathbf{u} \boldsymbol{\sigma}_k \mathbf{u}^{-1}\} \tag{9.7}$$

for all $\mathbf{u} \in \mathrm{SU}(2)$ and $j, k = 1, 2, 3$ (see Equations (2.9) and (2.10)). It is easily verified that ϕ is also analytic. Moreover, the kernel $\mathcal{K}$ is finite (consisting only of $\mathbf{1}_2$ and $-\mathbf{1}_2$), so that the mapping ψ of Equation (9.3) must be an isomorphic mapping.

Indeed both SU(2) and SO(3) are of dimension 3. Moreover, Equations (9.3) and (9.7) imply that for any $\mathbf{a} \in \mathcal{L}(=\mathrm{su}(2))$

$$\psi(\mathbf{a})_{jk} = (1/2)\mathrm{tr}\{\boldsymbol{\sigma}_j [\mathbf{a}, \boldsymbol{\sigma}_k]\}.$$

Consequently, with the basis $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ of $\mathcal{L}$ (=su(2)) defined by Equations (8.30), as $\mathbf{a}_j = \frac{1}{2} i \boldsymbol{\sigma}_j$ $(j = 1, 2, 3)$ and

$$[\boldsymbol{\sigma}_p, \boldsymbol{\sigma}_q] = \sum_{r=1}^{3} 2i\epsilon_{pqr}\boldsymbol{\sigma}_r$$

(where ϵ_{pqr} is defined by Equations (8.21)), it follows that $\psi(\mathbf{a}_p)_{jk} = \epsilon_{pjk}$. Thus

$$\psi(\mathbf{a}_1) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}, \quad \psi(\mathbf{a}_2) = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad \psi(\mathbf{a}_3) = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

These are precisely the basis elements of $\mathcal{L}' = \mathrm{so}(3)$ chosen in Equations (8.12). The isomorphic nature of ψ is confirmed by the fact that the commutation relations of so(3) (Equations (8.20)) and of su(2) (Equations (8.31)) are *identical*.

In this case both $\mathcal{G} = \mathrm{SU}(2)$ and $\mathcal{G}' = \mathrm{SO}(3)$ are compact. This point will be taken up again in Chapter 11, Section 10.

The only remaining case of interest is that in which $\mathcal{K}$ itself is a linear Lie group.

Theorem V Let $\mathcal{K}$ be the kernel of an analytic homomorphic mapping ϕ of a linear Lie group $\mathcal{G}$ of dimension n onto a linear Lie group $\mathcal{G}'$ of dimension n', and suppose that $\mathcal{K}$ is also a linear Lie group. Then $\mathcal{K}$ has dimension $(n - n')$ and its corresponding real Lie algebra is an invariant subalgebra of the real Lie algebra $\mathcal{L}$ of $\mathcal{G}$.

Proof Let $\mathcal{L}''$ be the real Lie algebra of $\mathcal{K}$. Theorem I of Section 2 implies that $\mathcal{L}''$ is an invariant subalgebra of $\mathcal{L}$ because $\mathcal{K}$ is an invariant subgroup

of $\mathcal{G}$. As ϕ maps the whole of $\mathcal{K}$ onto the identity of $\mathcal{G}'$, Equations (9.3) and (9.4) imply that a matrix $\mathbf{a}$ of $\mathcal{L}$ is a member of $\mathcal{L}''$ if and only if $\psi(\mathbf{a}) = \mathbf{0}$. Let $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n$ be a basis for $\mathcal{L}$ chosen so that $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_{n''}$ is a basis for $\mathcal{L}''$ (so that $\mathcal{L}''$ has dimension n''). Then $\psi(\mathbf{a}_j) = \mathbf{0}$ for $j = 1, 2, \ldots, n''$, while $\psi(\mathbf{a}_j)$ for $j = n'' + 1, n'' + 2, \ldots, n$ are linearly independent and so form a basis for $\mathcal{L}'$, the real Lie algebra of $\mathcal{G}'$. (For if $\alpha_{n''+1}, \ldots, \alpha_n$ are real numbers such that $\sum_{j=n''+1}^{n} \alpha_j \psi(\mathbf{a}_j) = \mathbf{0}$, then $\psi(\sum_{j=n''+1}^{n} \alpha_j \mathbf{a}_j) = \mathbf{0}$, implying that $\sum_{j=n''+1}^{n} \alpha_j \mathbf{a}_j \in \mathcal{L}''$ and hence $\alpha_{n''+1} = \ldots = \alpha_n = 0$.) Consequently $n' = n - n''$.

Hitherto the term "Lie subgroup" $\mathcal{G}'$ of a linear Lie group $\mathcal{G}$ has been used to describe a *subset* of $\mathcal{G}$ that is itself a linear Lie group (see Section 2 and Chapter 3, Section 1). Now suppose that $\mathcal{G}''$ is a linear Lie group that is analytically *isomorphic* to $\mathcal{G}'$. Although, strictly, $\mathcal{G}''$ is not a subgroup of $\mathcal{G}$ (as the elements of $\mathcal{G}''$ need not be members of $\mathcal{G}$), in practice very little confusion can arise if such a $\mathcal{G}''$ is described as being a Lie subgroup of $\mathcal{G}$. Indeed this looser usage is frequently encountered in the literature.

Example IV SU(2) *regarded as a Lie subgroup of* SU(3)
Suppose $\mathbf{u} \in \mathrm{SU}(2)$ and let

$$\phi(\mathbf{u}) = \begin{bmatrix} \mathbf{u} & \mathbf{0} \\ \mathbf{0} & 1 \end{bmatrix},$$

where the matrix on the right-hand side is a member of SU(3). Let $\mathcal{G}'$ denote the subset of elements of SU(3) that have this form. It is easily established that $\mathcal{G}'$ is a Lie subgroup of $\mathcal{G}$ in the strict sense and that ϕ is an analytic isomorphism of SU(2) onto $\mathcal{G}'$. Thus SU(2) can be regarded as being a Lie subgroup of SU(3).

4 Representations of Lie algebras

The definition of a representation and much of the subsequent discussion apply equally to real and complex Lie algebras.

Definition *Representation of a Lie algebra* $\mathcal{L}$
Suppose that to every $a \in \mathcal{L}$ there exists a $d \times d$ matrix $\mathbf{\Gamma}(a)$ such that

(i) for all $a, b \in \mathcal{L}$ and α, β of the field of $\mathcal{L}$

$$\mathbf{\Gamma}(\alpha a + \beta b) = \alpha \mathbf{\Gamma}(a) + \beta \mathbf{\Gamma}(b), \tag{9.8}$$

and

(ii) for all $a, b \in \mathcal{L}$

$$\mathbf{\Gamma}([a, b]) = [\mathbf{\Gamma}(a), \mathbf{\Gamma}(b)].$$

Then these matrices are said to form a "d-dimensional representation" of $\mathcal{L}$.

Clearly the set of matrices $\mathbf{\Gamma}(a)$ form a Lie algebra with the same field as $\mathcal{L}$ and there is a homomorphic mapping of $\mathcal{L}$ onto this Lie algebra. In specifying a representation of $\mathcal{L}$, it is obviously sufficient to specify *only* the matrices $\mathbf{\Gamma}(a_j)$ for every a_j of the basis of $\mathcal{L}$.

Many of the ideas on representations discussed in Chapter 4 for groups apply equally to Lie algebras. In particular, the duality between matrix representations and modules, the existence of similarity transformations and the concepts of reducible, completely reducible and irreducible representations re-appear.

Consider first the duality with modules (see Chapter 4, Section 1). If $\mathbf{\Gamma}$ is a d-dimensional representation of a Lie algebra $\mathcal{L}$, and $\psi_1, \psi_2, \ldots, \psi_d$ form the basis of a d-dimensional abstract complex inner product space V, the "carrier space", then for each $a \in \mathcal{L}$ an operator $\Phi(a)$ may be defined (cf. Equation (4.1)) by

$$\Phi(a)\psi_j = \sum_{k=1}^{d} \Gamma(a)_{kj}\psi_k, \; j = 1, 2, \ldots, d. \tag{9.9}$$

With the further definition that

$$\Phi(a)\{\sum_{j=1}^{d} b_j\psi_j\} = \sum_{j=1}^{d} b_j\{\Phi(a)\psi_j\}$$

for any set of complex numbers $b_1, b_2, \ldots, b_d$, it follows immediately that the set of operators $\Phi(a)$ form a Lie algebra and there is a homomorphic mapping of $\mathcal{L}$ onto this Lie algebra. Moreover, if the basis $\psi_1, \psi_2, \ldots, \psi_d$ of V is chosen to be an ortho-normal set, then (cf. Equation (4.4))

$$\Gamma(a)_{kj} = (\psi_k, \Phi(a)\psi_j)$$

for any $a \in \mathcal{L}$. Again the set of operators $\Phi(a)$ and the carrier space V are said to collectively form a "module".

Similarly, if $\mathbf{\Gamma}$ is a d-dimensional representation of $\mathcal{L}$ and $\mathbf{S}$ is any $d \times d$ non-singular matrix, then the set of matrices $\mathbf{\Gamma}'(a)$, defined for all $a \in \mathcal{L}$ by

$$\mathbf{\Gamma}'(a) = \mathbf{S}^{-1}\mathbf{\Gamma}(a)\mathbf{S},$$

also form a d-dimensional representation of $\mathcal{L}$. Again $\mathbf{\Gamma}$ and $\mathbf{\Gamma}'$ are said to be "equivalent" representations (see Chapter 4, Section 2).

Likewise, a d-dimensional representation of $\mathcal{L}$ is said to be "reducible" if it is equivalent to a representation $\mathbf{\Gamma}$ of $\mathcal{L}$ that can be partitioned in the form

$$\mathbf{\Gamma}(a) = \begin{bmatrix} \mathbf{\Gamma}_{11}(a) & \mathbf{\Gamma}_{12}(a) \\ \mathbf{0} & \mathbf{\Gamma}_{22}(a) \end{bmatrix} \tag{9.10}$$

for every $a \in \mathcal{L}$, the dimensions of the submatrices being as in Equation (4.8). A representation of $\mathcal{L}$ is then defined to be "irreducible" if it is not

reducible. Finally, a representation of $\mathcal{L}$ is said to be "*completely* reducible" it is equivalent to a representation $\mathbf{\Gamma}''$ of $\mathcal{L}$ that has the form

$$\mathbf{\Gamma}''(a) = \begin{bmatrix} \mathbf{\Gamma}''_{11}(a) & \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{\Gamma}''_{22}(a) & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{\Gamma}''_{33}(a) & \dots & \mathbf{0} \\ \vdots & \vdots & \vdots & & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{\Gamma}''_{rr}(a) \end{bmatrix} \tag{9.11}$$

for every $a \in \mathcal{L}$, where $\mathbf{\Gamma}''_{11}, \mathbf{\Gamma}''_{22}, \dots$ are all *irreducible* representations of $\mathcal{L}$. Because of the linear property of Equation (9.8), it is sufficient to consider only the matrices representing the basis elements of $\mathcal{L}$ when checking for reducibility or complete reducibility.

The name "Schur's Lemma" is also attached to one (or both) of the two following theorems.

Theorem I Let $\mathbf{\Gamma}$ and $\mathbf{\Gamma}'$ be two *irreducible* representations of a Lie algebra $\mathcal{L}$ of dimensions d and d' respectively, and suppose that there exists a $d \times d'$ matrix $\mathbf{A}$ such that $\mathbf{\Gamma}(a)\mathbf{A} = \mathbf{A}\mathbf{\Gamma}'(a)$ for all $a \in \mathcal{L}$. Then *either* $\mathbf{A} = \mathbf{0}$, *or* $d = d'$ and $\det \mathbf{A} \neq 0$.

Proof The proof given, for example, in Appendix C, Section 3, of Cornwell (1984) applies with the group $\mathcal{G}$ replaced by the Lie algebra $\mathcal{L}$. (Indeed the proof is applicable to any set of linear operators.)

Theorem II If $\mathbf{\Gamma}$ is a d-dimensional *irreducible* representation of a Lie algebra $\mathcal{L}$, and $\mathbf{B}$ is a $d \times d$ matrix such that $\mathbf{\Gamma}(a)\mathbf{B} = \mathbf{B}\mathbf{\Gamma}(a)$ for every $a \in \mathcal{L}$, then $\mathbf{B}$ must be a multiple of the unit matrix.

Proof This is exactly as for Theorem II of Chapter 4, Section 5, but with $\mathcal{G}$ replaced by $\mathcal{L}$.

As for groups, there is an immediate corollary for the Abelian situation.

Theorem III Every irreducible representation of an *Abelian* Lie algebra is *one*-dimensional.

Proof This is exactly as for Theorem III of Chapter 4, Section 5, but with $\mathcal{G}$ replaced by $\mathcal{L}$.

Of particular importance is the connection between the representations of a linear Lie group and those of its corresponding real Lie algebra. The transition from group to algebra is completely straightforward, as the following theorem shows, but the procedure does not necessarily work in the reverse direction.

Definition *Analytic representation of a linear Lie group* $\mathcal{G}$
Let $\mathbf{\Gamma}_{\mathcal{G}}$ be a representation of $\mathcal{G}$ in the abstract group sense (see Chapter 1,

Section 4) such that, for every $\mathbf{A}(x_1, x_2, \ldots, x_n) \in \mathcal{G}$ in some small neighbourhood of the identity of $\mathcal{G}$, the elements of $\mathbf{\Gamma}_{\mathcal{G}}(\mathbf{A}(x_1, x_2, \ldots, x_n))$ are *analytic* functions of $x_1, x_2, \ldots, x_n$ (in the sense of Chapter 3, Section 1). Then $\mathbf{\Gamma}_{\mathcal{G}}$ is said to be an "analytic representation" of $\mathcal{G}$.

Theorem IV Let $\mathbf{\Gamma}_{\mathcal{G}}$ be a d-dimensional analytic representation of a linear Lie group $\mathcal{G}$, whose corresponding real Lie algebra is $\mathcal{L}$.

(a) Then there exists a d-dimensional representation $\mathbf{\Gamma}_{\mathcal{L}}$ of $\mathcal{L}$ defined for each $\mathbf{a} \in \mathcal{L}$ by

$$\mathbf{\Gamma}_{\mathcal{L}}(\mathbf{a}) = [\tfrac{d}{dt}\mathbf{\Gamma}_{\mathcal{G}}(\exp(t\mathbf{a}))]_{t=0} \tag{9.12}$$

(b) For all $\mathbf{a} \in \mathcal{L}$ and all real t

$$\exp\{t\mathbf{\Gamma}_{\mathcal{L}}(\mathbf{a})\} = \mathbf{\Gamma}_{\mathcal{G}}(\exp(t\mathbf{a})). \tag{9.13}$$

(c) If $\mathbf{\Gamma}_{\mathcal{G}}$ and $\mathbf{\Gamma}'_{\mathcal{G}}$ are two d-dimensional analytic representations of $\mathcal{G}$ and $\mathbf{\Gamma}_{\mathcal{L}}$ and $\mathbf{\Gamma}'_{\mathcal{L}}$ are the associated representations of $\mathcal{L}$ defined as in Equation (9.12), then $\mathbf{\Gamma}_{\mathcal{L}}$ is equivalent to $\mathbf{\Gamma}'_{\mathcal{L}}$ if $\mathbf{\Gamma}_{\mathcal{G}}$ is equivalent to $\mathbf{\Gamma}'_{\mathcal{G}}$. The converse is also true if $\mathcal{G}$ is connected.

(d) $\mathbf{\Gamma}_{\mathcal{L}}$ is reducible if $\mathbf{\Gamma}_{\mathcal{G}}$ is reducible, and $\mathbf{\Gamma}_{\mathcal{L}}$ is completely reducible if $\mathbf{\Gamma}_{\mathcal{G}}$ is completely reducible. The converses are also true if $\mathcal{G}$ is connected.

(e) If $\mathcal{G}$ is connected then $\mathbf{\Gamma}_{\mathcal{L}}$ is irreducible if $\mathbf{\Gamma}_{\mathcal{G}}$ is irreducible. Conversely, $\mathbf{\Gamma}_{\mathcal{G}}$ is irreducible if $\mathbf{\Gamma}_{\mathcal{L}}$ is irreducible.

(f) If $\mathbf{\Gamma}_{\mathcal{G}}$ is a unitary representation, then $\mathbf{\Gamma}_{\mathcal{L}}(\mathbf{a})$ is anti-Hermitian for all $\mathbf{a} \in \mathcal{L}$. The converse is also true if $\mathcal{G}$ is connected.

Proof (a) and (b) The proofs are essentially the same as those of the corresponding parts of Theorem II of Section 3.
(c) Suppose that $\mathbf{\Gamma}'_{\mathcal{G}}(\mathbf{A}) = \mathbf{S}^{-1}\mathbf{\Gamma}_{\mathcal{G}}(\mathbf{A})\mathbf{S}$ for all $\mathbf{A} \in \mathcal{G}$. Then from Equations (9.12) and (9.13) and part (d) of Theorem III of Chapter 8, Section 2

$$\begin{aligned}
\mathbf{\Gamma}'_{\mathcal{L}}(\mathbf{a}) &= [\tfrac{d}{dt}\{\mathbf{S}^{-1}\mathbf{\Gamma}_{\mathcal{G}}(\exp(t\mathbf{a}))\mathbf{S}\}]_{t=0} \\
&= [\tfrac{d}{dt}\{\mathbf{S}^{-1}\exp\{t\mathbf{\Gamma}_{\mathcal{L}}(\mathbf{a})\}\mathbf{S}\}]_{t=0} \\
&= [\tfrac{d}{dt}\{\exp(t\mathbf{S}^{-1}\mathbf{\Gamma}_{\mathcal{L}}(\mathbf{a})\mathbf{S})\}]_{t=0} \\
&= \mathbf{S}^{-1}\mathbf{\Gamma}_{\mathcal{L}}(\mathbf{a})\mathbf{S}.
\end{aligned}$$

Conversely, if $\mathbf{\Gamma}'_{\mathcal{L}}(\mathbf{a}) = \mathbf{S}^{-1}\mathbf{\Gamma}_{\mathcal{L}}(\mathbf{a})\mathbf{S}$, then Equation (9.13) implies that

$$\mathbf{\Gamma}'_{\mathcal{G}}(\exp(t\mathbf{a})) = \mathbf{S}^{-1}\mathbf{\Gamma}_{\mathcal{G}}(\exp(t\mathbf{a}))\mathbf{S}.$$

Theorem VIII of Chapter 8, Section 5, then extends this result to the whole of $\mathcal{G}$ if $\mathcal{G}$ is connected.
(d) Equation (9.12) implies that $\mathbf{\Gamma}_{\mathcal{L}}$ is reducible if $\mathbf{\Gamma}_{\mathcal{G}}$ is reducible, and $\mathbf{\Gamma}_{\mathcal{L}}$

completely reducible if $\mathbf{\Gamma}_{\mathcal{G}}$ is completely reducible. Conversely, as every power of a matrix of the form in Equation (9.10) also has this form, so too has the exponential of such a matrix. The same is true of a matrix of the form in Equation (9.11). The converse results then follow from Equation (9.13) and Theorem VIII of Chapter 8, Section 5, provided that $\mathcal{G}$ is connected.
(e) This is an immediate consequence of (d).
(f) This follows from Equation (9.13), with Theorem VIII of Chapter 8, Section 5 being invoked in the converse proposition.

It is most important to realize that this theorem (and in particular Equation (9.13)) does *not* imply that every representation $\mathbf{\Gamma}_{\mathcal{L}}$ of $\mathcal{L}$ gives a representation of $\mathcal{G}$ by exponentiation. Rather, Equation (9.13) merely shows that *if* $\mathbf{\Gamma}_{\mathcal{G}}$ is an analytic representation of $\mathcal{G}$ *then* $\mathbf{\Gamma}_{\mathcal{G}}$ can be obtained from $\mathbf{\Gamma}_{\mathcal{L}}$ by exponentiation. The essential point is that, although the matrices $\exp\{t\mathbf{\Gamma}_{\mathcal{L}}(a)\}$ are well defined for all $\mathbf{a} \in \mathcal{L}$ and all real t, they do not necessarily form a representation of $\mathcal{G}$. The following examples will demonstrate this explicitly.

Example I *Connection between the representations of* $\mathcal{L} = \mathrm{so}(2)$ *and* $\mathcal{G} = \mathrm{SO}(2)$
$\mathcal{L} = \mathrm{so}(2)$ is one-dimensional. Let

$$\mathbf{a}_1 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

be its basis element (see Example II of Chapter 3, Section 1). As the only relevant commutation relation is the trivial one $[\mathbf{a}_1, \mathbf{a}_1] = \mathbf{0}$, it follows that $\mathbf{\Gamma}_{\mathcal{L}}(\mathbf{a}_1) = [p]$ provides a one-dimensional representation of $\mathcal{L}$ for *any* complex number p. Then $\exp\{t\mathbf{\Gamma}_{\mathcal{L}}(\mathbf{a}_1)\} = [\exp(tp)]$, while the elements of $\mathcal{G}$ have the form

$$\exp(t\mathbf{a}_1) = \begin{bmatrix} \cos t & \sin t \\ -\sin t & \cos t \end{bmatrix}.$$

However, $\exp((t + 2\pi)\mathbf{a}_1) = \exp(t\mathbf{a}_1)$, but

$$\exp\{(t + 2\pi)\mathbf{\Gamma}_{\mathcal{L}}(\mathbf{a}_1)\} = \exp(2\pi p)\exp\{t\mathbf{\Gamma}_{\mathcal{L}}(\mathbf{a}_1)\}.$$

Consequently this representation $\mathbf{\Gamma}_{\mathcal{L}}$ of $\mathcal{L}$ gives a representation of $\mathcal{G} = \mathrm{SO}(2)$ by exponentiation *if and only if* $p = iq$, where q is some integer.

Example II *Connection between the representations of* $\mathcal{L} = \mathrm{so}(3)$ *and* $\mathcal{G} = \mathrm{SO}(3)$
Let the matrices $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$ of Equations (8.12) provide a basis for $\mathcal{L} = \mathrm{so}(3)$. As demonstrated in Example II, so(3) is isomorphic to the real Lie algebra su(2). Thus a two-dimensional representation of $\mathcal{L} = \mathrm{so}(3)$ is provided by inverting the isomorphic mapping ψ of Example II, giving, by Equations (8.30),

$$\mathbf{\Gamma}_{\mathcal{L}}(\mathbf{a}_1) = \frac{1}{2}\begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix}, \quad \mathbf{\Gamma}_{\mathcal{L}}(\mathbf{a}_2) = \frac{1}{2}\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad \mathbf{\Gamma}_{\mathcal{L}}(\mathbf{a}_1) = \frac{1}{2}\begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}. \tag{9.14}$$

Then

$$\exp\{t\mathbf{\Gamma}_{\mathcal{L}}(\mathbf{a}_3)\} = \begin{bmatrix} \exp(\frac{1}{2}it) & 0 \\ 0 & \exp(-\frac{1}{2}it) \end{bmatrix},$$

while

$$\exp(t\mathbf{a}_3) = \begin{bmatrix} \cos t & \sin t & 0 \\ -\sin t & \cos t & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Thus $\exp\{(t+2\pi)\mathbf{a}_3\} = \exp(t\mathbf{a}_3)$, but $\exp\{(t+2\pi)\mathbf{\Gamma}_{\mathcal{L}}(\mathbf{a}_3)\} = -\exp\{t\mathbf{\Gamma}_{\mathcal{L}}(\mathbf{a}_3)\}$. Consequently the representation $\mathbf{\Gamma}_{\mathcal{L}}$ of $\mathcal{L} = \mathrm{so}(3)$ defined by Equation (9.13) *does not* on exponentiation give a representation of $\mathcal{G} = \mathrm{SO}(3)$. The question of which irreducible representations of $\mathcal{L} = \mathrm{so}(3)$ do provide representations of $\mathcal{G} = \mathrm{SO}(3)$ will be examined further in Chapter 10, Section 4.

Finally, there remains the question of the relationship between the *analytic* representations of a linear Lie group $\mathcal{G}$ defined above and the *continuous* representations of $\mathcal{G}$ introduced in Chapter 4, Section 1.

Theorem V If $\mathcal{G}$ is a compact linear Lie group then every continuous representation of $\mathcal{G}$ is analytic, and vice versa.

Proof See Naimark (1964). (The compactness of $\mathcal{G}$ comes in because invariant integration of $\mathcal{G}$ is necessary.)

It is worth noting that the continuity assumption was used in Chapter 4 *only* in the proofs of theorems for *compact* Lie groups, that is, precisely for those groups for which the concepts of continuity and analyticity are equivalent.

It is very useful to examine the connection between the representation of $\mathcal{G}$ and $\mathcal{L}$ in terms of modules. Denoting quantities associated with $\mathcal{G}$ and $\mathcal{L}$ by the appropriate subscripts, Equation (4.1) becomes (with $T = \exp(t\mathbf{a})$)

$$\Phi_{\mathcal{G}}(\exp(t\mathbf{a}))\psi_j = \sum_{k=1}^{d} \Gamma_{\mathcal{G}}(\exp(t\mathbf{a}))_{kj}\psi_k, \tag{9.15}$$

and Equation (9.9) becomes

$$\Phi_{\mathcal{L}}(\mathbf{a})\psi_j = \sum_{k=1}^{d} \Gamma_{\mathcal{L}}(\mathbf{a})_{kj}\psi_k. \tag{9.16}$$

Clearly Equations (9.12) and (9.13) imply that, for all $a \in \mathcal{L}$,

$$\Phi_{\mathcal{L}}(\mathbf{a}) = [\tfrac{d}{dt}\Phi_{\mathcal{G}}(\exp(t\mathbf{a}))]_{t=0}\ , \tag{9.17}$$

and

$$\exp\{t\Phi_{\mathcal{L}}(\mathbf{a})\} = \Phi_{\mathcal{G}}(\exp(t\mathbf{a})) \tag{9.18}$$

for all $\mathbf{a} \in \mathcal{L}$ and all real t. The linear operators $\Phi_{\mathcal{G}}(\exp(t\mathbf{a}))$ and $\Phi_{\mathcal{L}}(\mathbf{a})$ all operate in the *same* vector space V, and $\psi_1, \psi_2, \ldots, \psi_d$ form a basis *both* of $\mathbf{\Gamma}_{\mathcal{G}}$ *and* of $\mathbf{\Gamma}_{\mathcal{L}}$.

Of particular significance is the representation of $\mathcal{L}$ that corresponds to the direct product $\mathbf{\Gamma}^p \otimes \mathbf{\Gamma}^q$ of $\mathcal{G}$. Adding subscripts $\mathcal{G}$ to Equations (5.33) and (5.34) gives (for $T = \exp(t\mathbf{a})$)

$$\Phi_{\mathcal{G}}(\exp(t\mathbf{a}))\{\psi_j^p \otimes \psi_s^q\} = \{\Phi_{\mathcal{G}}^p(\exp(t\mathbf{a}))\psi_j^p\} \otimes \{\Phi_{\mathcal{G}}^q(\exp(t\mathbf{a}))\psi_s^q\} \tag{9.19}$$

and

$$\Phi_{\mathcal{G}}(\exp(t\mathbf{a}))\{\psi_j^p \otimes \psi_s^q\} = \sum_{k=1}^{d_p}\sum_{t=1}^{d_q}(\mathbf{\Gamma}_{\mathcal{G}}^p(\exp(t\mathbf{a})) \otimes (\mathbf{\Gamma}_{\mathcal{G}}^q(\exp(t\mathbf{a})))_{kt,js}\{\psi_k^p \otimes \psi_t^q\}, \tag{9.20}$$

where

$$\Phi_{\mathcal{G}}^p(\exp(t\mathbf{a}))\psi_j^p = \sum_{k=1}^{d_p}\Gamma_{\mathcal{G}}^p(\exp(t\mathbf{a}))_{kj}\psi_k^p \tag{9.21}$$

and

$$\Phi_{\mathcal{G}}^q(\exp(t\mathbf{a}))\psi_s^q = \sum_{t=1}^{d_q}\Gamma_{\mathcal{G}}^q(\exp(t\mathbf{a}))_{ts}\psi_t^q. \tag{9.22}$$

Thus, if $\mathbf{\Gamma}_{\mathcal{L}}^p$ and $\mathbf{\Gamma}_{\mathcal{L}}^q$ are the irreducible representations of $\mathcal{L}$ related to $\mathbf{\Gamma}_{\mathcal{G}}^p$ and $\mathbf{\Gamma}_{\mathcal{G}}^q$ by Equations (9.12) and (9.13) (with superscripts p and q added), and $\Phi_{\mathcal{L}}^p(\mathbf{a})$ and $\Phi_{\mathcal{L}}^q(\mathbf{a})$ are the corresponding linear operators (related to $\Phi_{\mathcal{G}}^p$ and $\Phi_{\mathcal{G}}^q$ by Equations (9.18) with superscripts p and q added), so that

$$\Phi_{\mathcal{L}}^p(\mathbf{a})\psi_j^p = \sum_{k=1}^{d_p}\Gamma_{\mathcal{L}}^p(\mathbf{a})_{kj}\psi_k^p \tag{9.23}$$

and

$$\Phi_{\mathcal{L}}^q(\mathbf{a})\psi_s^q = \sum_{t=1}^{d_q}\Gamma_{\mathcal{L}}^q(\mathbf{a})_{ts}\psi_t^q, \tag{9.24}$$

and if $\Phi_{\mathcal{L}}(\mathbf{a})$ are the linear operators corresponding to the $\Phi_{\mathcal{G}}$, then Equation (9.19) gives

$$\Phi_{\mathcal{L}}(\mathbf{a})\{\psi_j^p \otimes \psi_s^q\} = \{\Phi_{\mathcal{L}}^p(\mathbf{a})\psi_j^p\} \otimes \psi_s^q + \psi_j^p \otimes \{\Phi_{\mathcal{L}}^q(\mathbf{a})\psi_s^q\} \tag{9.25}$$

for all $\mathbf{a} \in \mathcal{L}$. Then, from Equations (9.23) and (9.24),

$$\Phi_{\mathcal{L}}(\mathbf{a})\{\psi_j^p \otimes \psi_s^q\} = \sum_{k=1}^{d_p}\sum_{t=1}^{d_q}(\mathbf{\Gamma}_{\mathcal{L}}^p(\mathbf{a}) \otimes \mathbf{1}_{d_q} + \mathbf{1}_{d_p} \otimes \mathbf{\Gamma}_{\mathcal{L}}^q(\mathbf{a}))_{kt,js}\{\psi_k^p \otimes \psi_t^q\} \tag{9.26}$$

for all $\mathbf{a} \in \mathcal{L}$, $j = 1, 2, \ldots, d_p$, and $s = 1, 2, \ldots, d_q$. Equation (9.26) shows that *the representation of* $\mathcal{L}$ *corresponding to the direct product representation* $\mathbf{\Gamma}^p \otimes \mathbf{\Gamma}^q$ *of* $\mathcal{G}$ *is given by the set of matrices*

$$\mathbf{\Gamma}_{\mathcal{L}}^p(\mathbf{a}) \otimes \mathbf{1}_{d_q} + \mathbf{1}_{d_p} \otimes \mathbf{\Gamma}_{\mathcal{L}}^q(\mathbf{a}). \tag{9.27}$$

Because the basis vectors of this representation are still the direct products of those of the two constituent representations, this representation of $\mathcal{L}$ will be called the "direct product" (or "Kronecker product") of the representations $\mathbf{\Gamma}^p_{\mathcal{L}}$ and $\mathbf{\Gamma}^q_{\mathcal{L}}$, and will be denoted symbolically by $\mathbf{\Gamma}^p_{\mathcal{L}} \otimes \mathbf{\Gamma}^q_{\mathcal{L}}$, even though its explicit form is not that of a straight direct product.

Further, as Equation (5.16) can be rewritten as

$$\mathbf{C}^{-1}\{\mathbf{\Gamma}^p_{\mathcal{G}}(\exp(t\mathbf{a})) \otimes \mathbf{\Gamma}^q_{\mathcal{G}}(\exp(t\mathbf{a}))\}\mathbf{C} = \sum_r \oplus n^r_{pq}\mathbf{\Gamma}^r_{\mathcal{G}}(\exp(t\mathbf{a})),$$

where $\mathbf{C}$ is the matrix of Clebsch-Gordan coefficients, it follows that

$$\mathbf{C}^{-1}\{\mathbf{\Gamma}^p_{\mathcal{L}}(\mathbf{a}) \otimes \mathbf{1}_{d_q} + \mathbf{1}_{d_p} \otimes \mathbf{\Gamma}^q_{\mathcal{L}}(\mathbf{a})\}\mathbf{C} = \sum_r \oplus n^r_{pq}\mathbf{\Gamma}^r_{\mathcal{L}}(\mathbf{a}).$$

Thus the irreducible representation $\mathbf{\Gamma}^r_{\mathcal{L}}$ of $\mathcal{L}$ appears n^r_{pq} times in the direct product of $\mathbf{\Gamma}^p_{\mathcal{L}}$ and $\mathbf{\Gamma}^q_{\mathcal{L}}$ *if* $\mathbf{\Gamma}^r_{\mathcal{G}}$ appears n^r_{pq} times in the direct product $\mathbf{\Gamma}^p_{\mathcal{G}} \otimes \mathbf{\Gamma}^q_{\mathcal{G}}$ of $\mathcal{G}$, and the reduction is performed using the *same* matrix of Clebsch-Gordan coefficients for *both* $\mathcal{G}$ and $\mathcal{L}$. Consequently, with $\theta^{r,\alpha}_l$ defined exactly as in Equation (5.35) by

$$\theta^{r,\alpha}_l = \sum_{j=1}^{d_p}\sum_{k=1}^{d_q} \left(\begin{array}{cc|cc} p & q & r, & \alpha \\ j & k & l & \end{array}\right) \psi^p_j \otimes \psi^q_k, \tag{9.28}$$

where $\left(\begin{array}{cc|cc} p & q & r, & \alpha \\ j & k & l & \end{array}\right)$ are the Clebsch-Gordan coefficients, then

$$\Phi_{\mathcal{L}}(\mathbf{a})\theta^{r,\alpha}_l = \sum_{u=1}^{d_r} \Gamma^r_{\mathcal{L}}(\mathbf{a})_{ul}\theta^{r,\alpha}_u \tag{9.29}$$

for all $\mathbf{a} \in \mathcal{L}$, $l = 1, 2, \ldots, d_r$ and $\alpha = 1, 2, \ldots, n^r_{pq}$, this being the Lie algebraic analogue of Equation (5.36). *It is important to note that the Clebsch-Gordan coefficients for the Lie group $\mathcal{G}$ and the real Lie algebra $\mathcal{L}$ are* **identical**.

These considerations can be generalized to *any* abstract Lie algebra $\mathcal{L}$, real or complex. As $\mathcal{L}$ need not be directly related to a linear Lie group, all the relevant concepts will be defined without reference to any group, and so the subscripts $\mathcal{L}$ of the previous analysis may be omitted. If $\Phi^p(a)$ and $\Phi^q(a)$ are the linear operators for $a \in \mathcal{L}$ of the irreducible representations $\mathbf{\Gamma}^p$ and $\mathbf{\Gamma}^q$ of $\mathcal{L}$, defined by

$$\left.\begin{array}{rcl} \Phi^p(a)\psi^p_j & = & \sum_{k=1}^{d_p} \Gamma^p(a)_{kj}\psi^p_k, \\ \Phi^q(a)\psi^q_s & = & \sum_{t=1}^{d_q} \Gamma^q(a)_{ts}\psi^q_t, \end{array}\right\} \tag{9.30}$$

then the operators $\Phi(a)$ corresponding to the "direct product" representation $\mathbf{\Gamma}^p \otimes \mathbf{\Gamma}^q$ of $\mathcal{L}$ will be defined (by analogy with Equation (9.25)) by

$$\Phi(a)\{\psi^p_j \otimes \psi^q_s\} = \{\Phi^p(a)\psi^p_j\} \otimes \psi^q_s + \psi^p_j \otimes \{\Phi^q(a)\psi^q_s\}, \tag{9.31}$$

for all $a \in \mathcal{L}$, $j = 1, 2, \ldots, d_p$, and $s = 1, 2, \ldots, d_q$. It is easily verified that $\Phi([a, a']) = [\Phi(a), \Phi(a')]$ for all $a, a' \in \mathcal{L}$. Then, by Equations (9.30) and (9.31),

$$\Phi(a)\{\psi_j^p \otimes \psi_s^q\} = \sum_{k=1}^{d_p} \sum_{t=1}^{d_q} (\mathbf{\Gamma}^p(a) \otimes \mathbf{1}_{d_q} + \mathbf{1}_{d_p} \otimes \mathbf{\Gamma}^q(a))_{kt,js} \{\psi_k^p \otimes \psi_t^q\}, \quad (9.32)$$

so the matrices $\mathbf{\Gamma}(a)$ defined by

$$\mathbf{\Gamma}(a) = \mathbf{\Gamma}^p(a) \otimes \mathbf{1}_{d_q} + \mathbf{1}_{d_p} \otimes \mathbf{\Gamma}^q(a) \quad (9.33)$$

form a $d_p d_q$-dimensional representation of $\mathcal{L}$ that will be called the "direct product" representation and denoted by $\mathbf{\Gamma}^p \otimes \mathbf{\Gamma}^q$. If the irreducible representation $\mathbf{\Gamma}^r$ of $\mathcal{L}$ appears n_{pq}^r times in $\mathbf{\Gamma}^p \otimes \mathbf{\Gamma}^q$ then the basis vectors $\theta_l^{r,\alpha}$ can again be expressed in the form of Equation (9.28), thereby defining Clebsch-Gordan coefficients of $\mathcal{L}$. As before, the matrix $\mathbf{C}$ of such coefficients reduces $\mathbf{\Gamma}^p \otimes \mathbf{\Gamma}^q$ of $\mathcal{L}$ into its irreducible constituents.

It is useful to express the definitions of irreducible tensor operators in Lie algebraic terms. For irreducible tensor operators of a linear Lie group $\mathcal{G}$ of coordinate transformations in $\mathbb{R}^3$, letting the transformation T of Equation (5.28) correspond to $\exp(t\mathbf{a})$, where $\mathbf{a}$ is an element of $\mathcal{L}$, the real Lie algebra associated with $\mathcal{G}$, and considering the limit as $t \to 0$ gives

$$[P(\mathbf{a}), Q_j^q] = \sum_{k=1}^{d_q} \Gamma^q(\mathbf{a})_{kj} Q_k^q, \quad (9.34)$$

which is valid for all $\mathbf{a} \in \mathcal{L}$ and $j = 1, 2, \ldots, d_q$. Here the operators $P(\mathbf{a})$ are as defined as in Equation (8.22). Similarly, for a general linear Lie group $\mathcal{G}$, Equation (5.37) gives

$$\Phi^r(\mathbf{a}) Q_j^q - Q_j^q \Phi^p(\mathbf{a}) = \sum_{k=1}^{d_q} \Gamma^q(\mathbf{a})_{kj} Q_k^q \quad (9.35)$$

for all $\mathbf{a}$ of the corresponding real Lie algebra $\mathcal{L}$ and $j = 1, 2, \ldots, d_q$. (Equation (9.35) can be taken as the definition of irreducible tensor operators for a general Lie algebra, modified if desired along the lines indicated in the last paragraph of Chapter 5, Section 4.)

5 The adjoint representations of Lie algebras and linear Lie groups

First the adjoint representation **ad** will be defined for a Lie algebra. (In Chapter 11, it will be shown that this representation plays a key role in the analysis of semi-simple Lie algebras.) Then the adjoint representation **Ad** of

a linear Lie group will be introduced and the connection between **ad** and **Ad** discussed.

Theorem I Let $\mathcal{L}$ be a real or complex Lie algebra of dimension n and let $a_1, a_2, \ldots, a_n$ be a basis for $\mathcal{L}$. For any $a \in \mathcal{L}$, let $\mathbf{ad}(a)$ be the $n \times n$ matrix defined by

$$[a, a_j] = \sum_{k=1}^{n} \{\mathbf{ad}(a)\}_{kj} a_k \tag{9.36}$$

for $j = 1, 2, \ldots, n$. Then the set of matrices $\mathbf{ad}(a)$ forms an n-dimensional representation of $\mathcal{L}$ called the "adjoint representation" of $\mathcal{L}$.

Proof See, for example, Chapter 11, Section 5, of Cornwell (1984).

Equations (9.36) and (8.18) together imply that

$$\{\mathbf{ad}(a_p)\}_{kj} = c_{pj}^{k} \tag{9.37}$$

for $j, k, p = 1, 2, \ldots, n$, where c_{pj}^{k} are the structure constants of $\mathcal{L}$. This in turn implies that, if $\mathcal{L}$ is a real Lie algebra, all the elements of $\mathbf{ad}(a)$ are real for all $a \in \mathcal{L}$.

It is occasionally convenient to use the corresponding *operators* $\mathrm{ad}(a)$, defined for each $a \in \mathcal{L}$ by

$$\mathrm{ad}(a)b = [a, b]$$

for all $b \in \mathcal{L}$. Then, by Equations (9.36),

$$\mathrm{ad}(a)a_j = \sum_{k=1}^{n} \{\mathbf{ad}(a)\}_{kj} a_k,$$

from which it follows by the preceding theorem that

$$\mathrm{ad}(\lambda a + \mu b) = \lambda \mathrm{ad}(a) + \mu \mathrm{ad}(b)$$

for all $a, b \in \mathcal{L}$ and all real or complex numbers λ, μ (as appropriate) and

$$\mathrm{ad}([a, b]) = [\mathrm{ad}(a), \mathrm{ad}(b)]$$

for all $a, b \in \mathcal{L}$.

Clearly the vector space on which the operators $\mathrm{ad}(a)$ act is $\mathcal{L}$ *itself*. The effect of taking a different basis $a_1', a_2', \ldots, a_n'$ instead of $a_1, a_2, \ldots, a_n$ is merely to induce a similarity transformation on the matrices $\mathbf{ad}(a)$. Indeed, with $a_p' = \sum_{q=1}^{n} S_{qp} a_q$, $\mathbf{ad}(a)$ is replaced by $\mathbf{S}^{-1}\mathbf{ad}(a)\mathbf{S}$ for each $a \in \mathcal{L}$.

Both the definition of the adjoint representation **Ad** of a linear Lie group $\mathcal{G}$ and certain results concerning the automorphisms of its corresponding real Lie algebra $\mathcal{L}$ depend on the following theorem.

Theorem II If $\mathcal{G}$ is a linear Lie group and $\mathcal{L}$ is its corresponding real Lie algebra, then, for any $\mathbf{A} \in \mathcal{G}$ and any $\mathbf{b} \in \mathcal{L}$, $\mathbf{AbA}^{-1}$ is a member of $\mathcal{L}$. Moreover, with $\mathbf{A} = \exp(t\mathbf{a})$, where $\mathbf{a} \in \mathcal{L}$,

$$\begin{aligned}\{\exp(t\mathbf{a})\}\,\mathbf{b}\,\{\exp(t\mathbf{a})\}^{-1} &= \mathbf{b} + t[\mathbf{a},\mathbf{b}] + \frac{1}{2}t^2[\mathbf{a},[\mathbf{a},\mathbf{b}]] \\ &\quad + \frac{1}{3!}t^3[\mathbf{a},[\mathbf{a},[\mathbf{a},\mathbf{b}]]] + \ldots \qquad (9.38)\end{aligned}$$

Proof Consider the set of elements $\mathbf{A}\{\exp(s\mathbf{b})\}\mathbf{A}^{-1}$ of $\mathcal{G}$, where $\mathbf{A} \in \mathcal{G}$, $\mathbf{b} \in \mathcal{L}$, and $-\infty < s < \infty$. They form a one-parameter subgroup of $\mathcal{G}$ whose generator is $\mathbf{AbA}^{-1}$, so that $\mathbf{AbA}^{-1} \in \mathcal{L}$.

Let $\mathbf{F}(t) = \{\exp(t\mathbf{a})\}\,\mathbf{b}\,\{\exp(t\mathbf{a})\}^{-1}$. Then $d\mathbf{F}/dt = [\mathbf{a},\mathbf{F}(t)]$, $d^2\mathbf{F}/dt^2 = [\mathbf{a},[\mathbf{a},\mathbf{F}(t)]]$ and so on. As the elements of $\mathbf{F}(t)$ are obviously analytic functions of t,

$$\begin{aligned}\mathbf{F}(t) &= \mathbf{F}(0) + t(d\mathbf{F}/dt)_{t=0} + \frac{1}{2}t^2(d^2\mathbf{F}/dt^2)_{t=0} + \ldots \\ &= \mathbf{b} + t[\mathbf{a},\mathbf{b}] + \frac{1}{2}t^2[\mathbf{a},[\mathbf{a},\mathbf{b}]] + \ldots\end{aligned}$$

Theorem III Let $\mathcal{G}$ be a linear Lie group of dimension n and let $\mathbf{a}_1$, $\mathbf{a}_2$, $\ldots$, $\mathbf{a}_n$ be a basis of its corresponding real Lie algebra $\mathcal{L}$. For each $\mathbf{A} \in \mathcal{G}$ let $\mathbf{Ad}(\mathbf{A})$ be the $n \times n$ matrix defined by

$$\mathbf{A}\mathbf{a}_j\mathbf{A}^{-1} = \sum_{k=1}^{n}\{\mathbf{Ad}(\mathbf{A})\}_{kj}\mathbf{a}_k \qquad (9.39)$$

for $j = 1, 2, \ldots, n$. Then

(a) the set of matrices $\mathbf{Ad}(\mathbf{A})$ forms an n-dimensional analytic representation of $\mathcal{G}$ called the "adjoint representation" of $\mathcal{G}$; and

(b) the associated representation of $\mathcal{L}$ defined by Equation (9.12) is the adjoint representation of $\mathcal{L}$; that is,

$$\mathbf{ad}(\mathbf{a}) = [\tfrac{d}{dt}\mathbf{Ad}(\exp(t\mathbf{a}))]_{t=0}$$

for any $\mathbf{a} \in \mathcal{L}$, so that for any $\mathbf{a} \in \mathcal{L}$ and all real t

$$\exp\{t\mathbf{ad}(\mathbf{a})\} = \mathbf{Ad}(\exp(t\mathbf{a})). \qquad (9.40)$$

Proof See, for example, Chapter 11, Section 5, of Cornwell (1984).

This is a convenient point to derive a useful result concerning the automorphisms of a real Lie algebra.

Theorem IV Let $\mathcal{G}$ be a connected linear Lie group and $\mathcal{L}$ its corresponding real Lie algebra. Then, for any $\mathbf{A} \in \mathcal{G}$, the mapping $\psi_{\mathbf{A}}$ of $\mathcal{L}$ onto itself, defined by

$$\psi_{\mathbf{A}}(\mathbf{b}) = \mathbf{A}\mathbf{b}\mathbf{A}^{-1} \tag{9.41}$$

for all $\mathbf{b} \in \mathcal{L}$, is an *automorphism* of $\mathcal{L}$ and is called an "inner automorphism" of $\mathcal{L}$.

Proof Theorem II of this section shows that $\psi_{\mathbf{A}}$ is definitely a mapping of $\mathcal{L}$ into itself. Moreover, for any $\mathbf{b}' \in \mathcal{L}$ there exists a $\mathbf{b} \in \mathcal{L}$ (namely $\mathbf{b} = \mathbf{A}^{-1}\mathbf{b}'\mathbf{A}$) such that $\psi_{\mathbf{A}}(\mathbf{b}) = \mathbf{b}'$, and the mapping is obviously one-to-one. The linear requirement of Equation (9.1) is trivially satisfied, while for any $\mathbf{b}, \mathbf{b}' \in \mathcal{L}$

$$\begin{aligned} \psi_{\mathbf{A}}([\mathbf{b}, \mathbf{b}']) &= \mathbf{A}(\mathbf{b}\mathbf{b}' - \mathbf{b}'\mathbf{b})\mathbf{A}^{-1} = \mathbf{A}\mathbf{b}\mathbf{A}^{-1}\mathbf{A}\mathbf{b}'\mathbf{A}^{-1} - \mathbf{A}\mathbf{b}'\mathbf{A}^{-1}\mathbf{A}\mathbf{b}\mathbf{A}^{-1} \\ &= [\psi_{\mathbf{A}}(\mathbf{b}), \psi_{\mathbf{A}}(\mathbf{b}')], \end{aligned}$$

so that Equation (9.2) is also satisfied.

The set of all inner automorphisms of $\mathcal{L}$ will be denoted by $\mathrm{Int}(\mathcal{L})$. As $\mathrm{Int}(\mathcal{L})$ is the connected component of $\mathrm{Aut}(\mathcal{L})$, the group of all automorphisms of $\mathcal{L}$, it follows that $\mathrm{Int}(\mathcal{L})$ must be an *invariant* subgroup of $\mathrm{Aut}(\mathcal{L})$.

6 Direct sum of Lie algebras

Again the basic definition applies both to real and complex Lie algebras.

Definition *Direct sum of two Lie algebras*
A Lie algebra $\mathcal{L}$ is said to be the "direct sum" of two Lie algebras $\mathcal{L}_1$ and $\mathcal{L}_2$ (all with the same field) if

(i) the vector space of $\mathcal{L}$ is the direct sum of the vector spaces of $\mathcal{L}_1$ and $\mathcal{L}_2$ (see Appendix B, Section 1), and

(ii) for all $a' \in \mathcal{L}_1$ and $a'' \in \mathcal{L}_2$, $[a', a''] = 0$.

This is expressed by writing $\mathcal{L} = \mathcal{L}_1 \oplus \mathcal{L}_2$.

The concept can be clarified by expressing it in terms of the basis elements of $\mathcal{L}_1$, $\mathcal{L}_2$ and $\mathcal{L}$. Let $a_1, a_2, \ldots, a_n$ be a basis for $\mathcal{L}$ constructed in such a way that $a_1, a_2, \ldots, a_{n_1}$ is a basis for $\mathcal{L}_1$ and $a_{n_1+1}, a_{n_1+2}, \ldots, a_n$ is a basis for $\mathcal{L}_2$. If $[a_p, a_q] = 0$ for $p = 1, 2, \ldots, n_1$ and $q = n_1 + 1, n_1 + 2, \ldots, n$, then $\mathcal{L} = \mathcal{L}_1 \oplus \mathcal{L}_2$. Obviously the dimension of $\mathcal{L}$ is the sum of the dimensions of $\mathcal{L}_1$ and $\mathcal{L}_2$. It is clear that $\mathcal{L}_1 \oplus \mathcal{L}_2$ can be constructed for *any* two Lie algebras $\mathcal{L}_1$ and $\mathcal{L}_2$ having the same field.

The relationship of this concept for real Lie algebras to that of direct products of linear Lie groups is succinctly expressed in the following theorem.

Theorem I If $\mathcal{G}_1$ and $\mathcal{G}_2$ are two linear Lie groups of dimensions n_1 and n_2 respectively, then $\mathcal{G}_1 \otimes \mathcal{G}_2$ is a linear Lie group of dimension $(n_1 + n_2)$. Moreover, if $\mathcal{L}_1$ and $\mathcal{L}_2$ are the real Lie algebras of $\mathcal{G}_1$ and $\mathcal{G}_2$, then the real Lie algebra of $\mathcal{G}_1 \otimes \mathcal{G}_2$ is isomorphic to $\mathcal{L}_1 \oplus \mathcal{L}_2$.

Proof See, for example, Chapter 11, Section 6, of Cornwell (1984).

This theorem shows that there always exists a direct product group whose real Lie algebra is isomorphic to $\mathcal{L}_1 \oplus \mathcal{L}_2$. However, *not every* linear Lie group with real Lie algebra isomorphic to $\mathcal{L}_1 \oplus \mathcal{L}_2$ is a direct product group, as the following example shows.

Example I $\mathcal{G} = \mathrm{U}(2)$ *and its direct sum real Lie algebra*
As noted in Table 8.1, the real Lie algebra $\mathcal{L} = \mathrm{u}(2)$ of $\mathcal{G} = \mathrm{U}(2)$ is the set of all 2×2 anti-Hermitian matrices (which need not be traceless). Thus a convenient basis of u(2) is provided by the matrices $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ of Equations (8.30), together with $\mathbf{a}_4 = i\mathbf{1}_2$. Clearly $[\mathbf{a}_p, \mathbf{a}_4] = \mathbf{0}$ for $p = 1, 2, 3$, so $\mathcal{L} = \mathrm{u}(2)$ is the direct sum of a real Lie algebra $\mathcal{L}_1$, with basis $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$, and a real Lie algebra $\mathcal{L}_2$ with basis $\mathbf{a}_4$.

Let $\mathcal{G}_1$ and $\mathcal{G}_2$ be the linear Lie groups obtained by exponentiating the matrices of $\mathcal{L}_1$ and $\mathcal{L}_2$. As $\mathcal{L}_1 = \mathrm{su}(2)$, it follows that $\mathcal{G}_1 = \mathrm{SU}(2)$, while $\mathcal{G}_2$ is clearly the set of matrices $\exp(it)\mathbf{1}_2$ for all real t. Although $\mathcal{G}_1$ and $\mathcal{G}_2$ are both subgroups of $\mathcal{G} = \mathrm{U}(2)$ and the elements of $\mathcal{G}_1$ commute with those of $\mathcal{G}_2$, nevertheless $\mathcal{G}$ is *not* isomorphic to $\mathcal{G}_1 \otimes \mathcal{G}_2$. The reason is that $\mathcal{G}_1$ and $\mathcal{G}_2$ possess *two* common elements, namely $\mathbf{1}_2$ and $-\mathbf{1}_2$, so that the fourth necessary condition of Theorem II of Chapter 2, Section 7, is *not* satisfied.

A very similar argument applied to $\mathrm{U}(N)$ for $N = 3, 4, 5, \ldots$ shows that $\mathrm{U}(N)$ is *not* isomorphic to $\mathrm{SU}(N) \otimes \mathrm{U}(1)$, even though $\mathrm{u}(N) = \mathrm{su}(N) \oplus \mathrm{u}(1)$.

The close connection with direct product groups means that all the results on representations of direct product groups discussed in Chapter 5, Section 5, have Lie algebraic analogues.

The fact that representations of the direct product $\mathcal{G}_1 \otimes \mathcal{G}_2$ of two linear Lie groups $\mathcal{G}_1$ and $\mathcal{G}_2$ are given by the direct products of the representations of $\mathcal{G}_1$ and $\mathcal{G}_2$, that $\mathcal{L}_1 \oplus \mathcal{L}_2$ is the real Lie algebra of $\mathcal{G}_1 \otimes \mathcal{G}_2$, and that the Lie algebraic version of a direct product representation is given by Expression (9.27) all combine to suggest the following theorems.

Theorem II Let $\mathbf{\Gamma}_1$ and $\mathbf{\Gamma}_2$ be representations of dimensions d_1 and d_2 of two Lie algebras $\mathcal{L}_1$ and $\mathcal{L}_2$ respectively (where $\mathcal{L}_1$ and $\mathcal{L}_2$ are either both real or both complex). Then the set of matrices defined

$$\mathbf{\Gamma}(a' + a'') = \mathbf{\Gamma}_1(a') \otimes \mathbf{1}_{d_2} + \mathbf{1}_{d_1} \otimes \mathbf{\Gamma}_2(a'') \tag{9.42}$$

for all $a' \in \mathcal{L}_1$ and $a'' \in \mathcal{L}_2$ provides a $d_1 d_2$-dimensional representation of $\mathcal{L}_1 \oplus \mathcal{L}_2$.

Proof If $a', b' \in \mathcal{L}_1$ and $a'', b'' \in \mathcal{L}_2$, then Equation (9.42) gives

$$\begin{aligned}
&[\mathbf{\Gamma}(a' + a''), \mathbf{\Gamma}(b' + b'')] \\
&= [\{\mathbf{\Gamma}_1(a') \otimes \mathbf{1}_{d_2} + \mathbf{1}_{d_1} \otimes \mathbf{\Gamma}_2(a'')\}, \{\mathbf{\Gamma}_1(b') \otimes \mathbf{1}_{d_2} + \mathbf{1}_{d_1} \otimes \mathbf{\Gamma}_2(b'')\}] \\
&= [\mathbf{\Gamma}_1(a'), \mathbf{\Gamma}_1(b')] \otimes \mathbf{1}_{d_2} + \mathbf{1}_{d_1} \otimes [\mathbf{\Gamma}_2(a''), \mathbf{\Gamma}_2(b'')] \\
&= \mathbf{\Gamma}_1([a', b']) \otimes \mathbf{1}_{d_2} + \mathbf{1}_{d_1} \otimes [\mathbf{\Gamma}_2([a'', b''])] \\
&= \mathbf{\Gamma}([(a' + a''), (b' + b'')])
\end{aligned}$$

Theorem III If $\mathcal{L}_1$ and $\mathcal{L}_2$ are the real Lie algebras of two compact linear Lie groups and $\mathbf{\Gamma}_1$ and $\mathbf{\Gamma}_2$ are irreducible representations of $\mathcal{L}_1$ and $\mathcal{L}_2$ respectively, then the representation $\mathbf{\Gamma}$ defined by Equation (9.42) is an *irreducible* representation of $\mathcal{L}_1 \oplus \mathcal{L}_2$. Moreover, *every* irreducible representation of $\mathcal{L}_1 \oplus \mathcal{L}_2$ is equivalent to a representation constructed in this way.

Proof This follows immediately from the corresponding result for direct products of compact Lie groups (given as Theorem II of Chapter 5, Section 5) and the results of Section 4.

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Chapter 10

The Three-dimensional Rotation Groups

1 Some properties reviewed

When the rotation groups in $\mathbb{R}^3$ were first introduced in Chapter 1, Section 2(a), it was noted immediately that the group of all rotations in $\mathbb{R}^3$ is isomorphic to O(3) and its subgroup of all proper rotations is isomorphic to SO(3). Example I of Chapter 2, Section 7, demonstrated that O(3) is just the direct product of SO(3) with the group of order 2 consisting of the identity and the spatial inversion matrix. It was also noted (in Chapter 2, Section 6) that there is a homomorphic mapping of SU(2) onto SO(3), which is responsible for the isomorphism that exists between their corresponding real Lie algebras su(2) and so(3) (as was demonstrated in detail in Example III of Chapter 9, Section 3).

The properties of SO(3), O(3), SU(2) and the rotation groups of $\mathbb{R}^3$ will now be investigated in detail. The conjugacy classes of these groups will be studied in Section 2. Then, in Section 3, the irreducible representations of the isomorphic Lie algebras su(2) and so(3) will be derived. These are of great importance not merely for their immediate physical applications but also because they play an essential part in the analysis of the representations of any semi-simple Lie algebra. When the irreducible representations of the corresponding groups are examined in the next section, attention will be drawn to the fact that every irreducible representation of su(2) exponentiates to give an irreducible representation of SU(2), but this representation of SU(2) may or may not provide a representation of SO(3). The irreducible representations of both SO(3) and O(3) will be identified. The Clebsch-Gordan series and coefficients are discussed briefly in Section 5. Finally some applications in atomic physics are described in Section 6. The close connection with the theory of angular momentum in quantum mechanics appears as a constantly recurring theme.

2 The class structures of SU(2) and SO(3)

It is useful to have another parametrization of SO(3) and SU(2). Let T be the proper rotation through an angle ω in the right-hand screw sense about an axis that lies in the direction of the unit vector $\mathbf{n} = (n_1, n_2, n_3)$. Then the transformation matrix $\mathbf{R}(T)$ is given by

$$R(T)_{jk} = \delta_{jk}\cos\omega + n_j n_k(1-\cos\omega) + \sin\omega \sum_{l=1}^{3} \epsilon_{jkl} n_l \tag{10.1}$$

(for $j, k = 1, 2, 3$), where ϵ_{jkl} is the permutation symbol defined in Equations (8.21). It is convenient to adopt the convention that ω is allowed to take any value in the interval $-\pi < \omega \leq \pi$, which implies that if $\mathbf{n}$ is an allowed unit vector then $-\mathbf{n}$ is not permitted. (For example, the possible values of the components of $\mathbf{n}$ could be restricted so that $n_3 > 0$, or if $n_3 = 0$ then $n_2 > 0$, or if $n_3 = 0$ and $n_2 = 0$ then $n_1 = 1$. With this convention a negative value of ω corresponds to a rotation in the left-hand screw sense.) The corresponding element $\mathbf{u}$ of SU(2) is then given by

$$\mathbf{u} = \mathbf{1}\cos(\omega/2) + i\{n_1\boldsymbol{\sigma}_1 + n_2\boldsymbol{\sigma}_2 + n_3\boldsymbol{\sigma}_3\}\sin(\omega/2), \tag{10.2}$$

where $\boldsymbol{\sigma}_1$, $\boldsymbol{\sigma}_2$ and $\boldsymbol{\sigma}_3$ are the Pauli spin matrices of Equations (2.10). Here $\mathbf{n}$ is restricted as above, but ω will be allowed to take any value in the interval $-2\pi < \omega \leq 2\pi$. (The two-valued nature of the homomorphic mapping of SU(2) onto SO(3) is reflected in the fact that ω and $\omega + 2\pi$ correspond to the same proper rotation $\mathbf{R}(T)$ while giving matrices $\mathbf{u}$ with opposite signs.) The matrix $\mathbf{u}$ defined in Equation (10.2) will be said to "correspond to the rotation ω about the axis $\mathbf{n}$ $(-2\pi < \omega \leq 2\pi)$". (The proofs of Equations (10.1) and (10.2) may be found, for example, in Chapter 12, Section 2, of Cornwell (1984)).

Rewriting Equation (10.1) in full,

$$\mathbf{R}(T) = \begin{bmatrix} \cos\omega + n_1^2(1-\cos\omega) & n_1n_2(1-\cos\omega) + n_3\sin\omega & n_1n_3(1-\cos\omega) - n_2\sin\omega \\ n_1n_2(1-\cos\omega) - n_3\sin\omega & \cos\omega + n_2^2(1-\cos\omega) & n_2n_3(1-\cos\omega) + n_1\sin\omega \\ n_1n_3(1-\cos\omega) + n_2\sin\omega & n_2n_3(1-\cos\omega) - n_1\sin\omega & \cos\omega + n_3^2(1-\cos\omega) \end{bmatrix}. \tag{10.3}$$

Thus, as $\sum_{j=1}^{3} n_j^2 = 1$,

$$\operatorname{tr}\mathbf{R}(T) = 1 + 2\cos\omega. \tag{10.4}$$

These results lead to the main conclusion of this section:

Theorem I Two elements of SU(2) belong to the same class of SU(2) if and only if they correspond to rotations having the same value of $|\omega|$. Similarly, two proper rotations in $\mathbb{R}^3$ belong to the same class of the group of all proper rotations in $\mathbb{R}^3$ if and only if they have the same value of $|\omega|$. Finally, two rotations of the group of all rotations in $\mathbb{R}^3$ are in the same class of that

group if and only if both rotations are proper or both are improper and the proper parts have the same value of $|\omega|$.

Proof For details, see, for example, Chapter 12, Section 2, of Cornwell (1984).

It should be pointed out that this theorem applies to the group of all *proper* rotations in $\mathbb{R}^3$ and to the group of *all* rotations in $\mathbb{R}^3$. For proper subgroups of these groups it is possible to have two rotations of the same type (that is, both corresponding to the same value of $|\omega|$ and both proper or both improper) lying in *different* classes, as was discussed in detail in Chapter 2, Section 2.

It follows from this theorem that, in all representations of SU(2) and of SO(3), the *characters* depend *only* on the value of $|\omega|$ and not on the direction $\mathbf{n}$ that specifies the axis of rotation.

For $\mathbf{n}$ *fixed* the set of rotations T whose transformation matrices $\mathbf{R}(T)$ are given by Equation (10.3) clearly form a one-parameter subgroup, the parameter being ω. This subgroup is generated by the 3×3 matrix $\mathbf{a}$, such that

$$\mathbf{a} = \lim_{\omega \to 0} \{\mathbf{R}(T) - \mathbf{1}\}/\omega.$$

Thus, from Equation (10.3),

$$\mathbf{a} = \begin{bmatrix} 0 & n_3 & -n_2 \\ -n_3 & 0 & n_1 \\ n_2 & -n_1 & 0 \end{bmatrix},$$

so that

$$\mathbf{a} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_2\mathbf{a}_2,$$

where $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ are the basis elements of the Lie algebra so(3) defined by Equations (8.12). Thus $n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_2\mathbf{a}_2$ *generates a one-parameter subgroup of proper rotations about the axis specified by the unit vector* $\mathbf{n} = (n_1, n_2, n_3)$.

3 Irreducible representations of the Lie algebras su(2) and so(3)

The intimate connection between the isomorphic Lie algebras su(2) and so(3) and the algebra of quantum mechanical angular momentum operators was noted in Chapter 8, Section 4. It should come as no surprise that the argument that will now be given for determining the irreducible representations of su(2) and so(3) is essentially that which gives the eigenvalues and eigenvectors of the angular momentum operators and which appears in many books on quantum mechanics (e.g. Schiff 1968).

As su(2) and so(3) are isomorphic they have the same representations. The following arguments will be given for su(2), but naturally they apply equally to so(3). As the basis elements in Equations (8.30) of su(2) are linearly independent over the field of complex numbers, the complexification $\widetilde{\mathcal{L}}$

of su(2) can be taken to be the complex vector space consisting of complex linear combinations of the basis elements $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$ of su(2), their basic commutation relations remaining as in Equations (8.31). ($\widetilde{\mathcal{L}}$ is denoted by A_1 in the Cartan classification of simple complex Lie algebras given in Chapter 11.) Essentially the following argument produces the irreducible representations of $\widetilde{\mathcal{L}}$, from which those of su(2) follow immediately as $\widetilde{\mathcal{L}}$ and su(2) have the same basis elements.

As the Lie group SU(2) is compact, each irreducible representation of SU(2) can be taken to be unitary. Part (f) of Theorem IV of Chapter 9, Section 4, shows that the corresponding representations of su(2) consist of anti-Hermitian matrices. Thus if $\psi_1, \psi_2, \ldots, \psi_d$ is an ortho-normal basis of such a d-dimensional representation $\mathbf{\Gamma}$ of su(2) in an inner product space V and the linear operators $\Phi(a)$ are defined for all a of su(2) by

$$\Phi(\mathbf{a})\psi_p = \sum_{q=1}^{d} \Gamma(\mathbf{a})_{qp}\psi_q, \quad p = 1, 2, \ldots, d, \tag{10.5}$$

then, as $(\psi_q, \Phi(\mathbf{a})\psi_p) = \Gamma(\mathbf{a})_{qp} = -\Gamma(\mathbf{a})^*_{pq} = -(\Phi(\mathbf{a})\psi_q, \psi_p)$, it follows that

$$(\phi, \Phi(\mathbf{a})\psi) = -(\Phi(\mathbf{a})\phi, \psi) \tag{10.6}$$

for all $\phi, \psi \in V$ and all $\mathbf{a} \in$ su(2). It is therefore convenient to define three linear operators A_1, A_2, A_3 by

$$A_p = -i\Phi(\mathbf{a}_p), \quad p = 1, 2, 3 \tag{10.7}$$

so that, by Equation (10.6),

$$(\phi, A_p\Psi) = (A_p\phi, \psi) \tag{10.8}$$

for all $\phi, \psi \in V$ and $p = 1, 2, 3$. That is, A_1, A_2, A_3 are *self-adjoint* operators. Also, as $[\Phi(\mathbf{a}_p), \Phi(\mathbf{a}_q)] = \Phi([\mathbf{a}_p, \mathbf{a}_q])$, Equations (8.31) give

$$[A_p, A_q] = i\sum_{r=1}^{3} \epsilon_{pqr}A_r, \quad p, q = 1, 2, 3, \tag{10.9}$$

where ϵ_{pqr} is the permutation symbol of Equations (8.21).

Now define the "ladder operators" A_+ and A_- by

$$A_+ = A_1 + iA_2, \; A_- = A_1 - iA_2, \tag{10.10}$$

so that

$$A_1 = (A_+ + A_-)/2, \; A_2 = -i(A_+ - A_-)/2. \tag{10.11}$$

Then, by Equation (10.9),

$$[A_3, A_+] = A_+, \tag{10.12}$$

$$[A_3, A_-] = -A_-, \tag{10.13}$$

$$[A_+, A_-] = 2A_3. \tag{10.14}$$

Moreover, Equation (10.8) implies that

$$(A_-\phi, \psi) = (\phi, A_+\psi) \tag{10.15}$$

for all $\phi, \psi \in V$.

Finally, define the operator A^2 by

$$A^2 = A_1^2 + A_2^2 + A_3^2. \tag{10.16}$$

Then, by Equation (10.9),

$$[A^2, A_p] = 0, \quad p = 1, 2, 3, \tag{10.17}$$

which in turn implies that

$$[A^2, A_+] = [A^2, A_-] = 0. \tag{10.18}$$

Also, as $A_-A_+ = (A_1 - iA_2)(A_1 + iA_2) = A_1^2 + A_2^2 + i[A_1, A_2]$, Equations (10.9) and (10.16) give

$$A_-A_+ = A^2 - A_3^2 - A_3. \tag{10.19}$$

Similarly,

$$A_+A_- = A^2 - A_3^2 + A_3. \tag{10.20}$$

In the quantum mechanical theory of angular momentum, the operators J_x, J_y, J_z corresponding to the components about Ox, Oy and Oz satisfy the commutation relations

$$[J_x, J_y] = i\hbar J_z, \ [J_y, J_z] = i\hbar J_x, \ [J_z, J_x] = i\hbar J_y. \tag{10.21}$$

J_x, J_y and J_z are general angular momentum operators, in the sense that they may correspond to intrinsic spin, orbital angular momentum, or a combination of both. The symbols L_x, L_y and L_z will be reserved for the special case of orbital angular momentum (as in Chapter 8, Section 4). Apart from a factor $\hbar$, Equations (10.9) and (10.21) are identical. Therefore the identifications

$$\left.\begin{array}{lllllll} J_x & = & \hbar A_1, & J_y & = & \hbar A_2, & J_z = \hbar A_3, \\ J_+ & = & \hbar A_+, & J_- & = & \hbar A_-, & \\ J^2 & = & \hbar^2 A^2, & & & & \end{array}\right\} \tag{10.22}$$

provide the connection between the representation theory of su(2) and the theory of angular momentum.

Returning to su(2), in any representation $\mathbf{\Gamma}$ of $\widetilde{\mathcal{L}}$ the matrix representing A^2 (defined by $\mathbf{\Gamma}(A^2) = \sum_{p=1}^{3}\{\mathbf{\Gamma}(A_p)\}^2$) commutes (by Equation (10.17)) with $\mathbf{\Gamma}(\mathbf{a})$ for all $\mathbf{a} \in \widetilde{\mathcal{L}}$. Schur's Lemma (see Chapter 9, Section 4) then implies that if $\mathbf{\Gamma}$ is *irreducible* then $\mathbf{\Gamma}(A^2)$ must be a multiple of the unit matrix, so all the basis vectors $\psi_1, \psi_2, \ldots, \psi_d$ of V are eigenvectors of A^2 with the *same* eigenvalue.

It is convenient to summarize the main conclusions concerning the irreducible representations of su(2) in the form of a theorem. The results have immediate application in the theory of angular momentum and the theory of isotopic spin, as well as forming the basis of the representation theory of semi-simple Lie algebras that will be developed in Chapter 12.

Theorem I To every non-negative integer or half-integer j (i.e. for $j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$) there exists an irreducible representation of su(2) (and its complexification A_1) of dimension $d = 2j + 1$. The ortho-normal basis vectors of the irreducible representation specified by j may be denoted by ψ^j_m, where m takes all values from j down to $-j$ in integral steps (i.e. $m = j, j-1, j-2, \ldots, -j+1, -j$). Each basis vector ψ^j_m may be chosen to be a simultaneous eigenvector of A^2 and A_3 with eigenvalues $j(j+1)$ and m respectively, that is

$$A^2\psi^j_m = j(j+1)\psi^j_m, \tag{10.23}$$

$$A_3\psi^j_m = m\psi^j_m, \tag{10.24}$$

(for $m = j, j-1, \ldots, -j$). Moreover, the relative phases of the basis vectors may be chosen so that

$$A_+\psi^j_m = \{(j-m)(j+m+1)\}^{1/2}\psi^j_{m+1}, \tag{10.25}$$

$$A_-\psi^j_m = \{(j+m)(j-m+1)\}^{1/2}\psi^j_{m-1}, \tag{10.26}$$

for $m = j, j-1, \ldots, -j$. Up to equivalence these are the only irreducible representations of su(2) (and its complexification A_1).

The matrices of this irreducible representation may be denoted by $\mathbf{D}^j(\mathbf{a})$, with elements $D^j(\mathbf{a})_{m'm}$, where m' and m take the values $j, j-1, \ldots, -j+1, -j$ (these all being integers if j is an integer and all being half-integers if j is a half-integer). Then

$$\left.\begin{aligned} D^j(\mathbf{a}_1)_{m'm} &= \tfrac{1}{2}i[\delta_{m',m+1}\{(j-m)(j+m+1)\}^{1/2} \\ &\quad +\delta_{m',m-1}\{(j+m)(j-m+1)\}^{1/2}], \\ D^j(\mathbf{a}_2)_{m'm} &= \tfrac{1}{2}[\delta_{m',m+1}\{(j-m)(j+m+1)\}^{1/2} \\ &\quad -\delta_{m',m-1}\{(j+m)(j-m+1)\}^{1/2}], \\ D^j(\mathbf{a}_3)_{m'm} &= im\delta_{m',m}\,. \end{aligned}\right\} \tag{10.27}$$

Proof By an appropriate similarity transformation, each irreducible representation $\mathbf{\Gamma}$ of su(2) may be chosen so that the matrix representing $\mathbf{a}_3$ is diagonal. This implies that the basis vectors may all be chosen to be eigenvectors of A_3, as well as being eigenvectors of A^2. As A_3 is self-adjoint, all its eigenvalues are real. Let ψ denote an eigenvector of A_3 with eigenvalue m (so that $A_3\psi = m\psi$). Then, by Equation (10.12), $A_3(A_+\psi) = (m+1)(A_+\psi)$, so $A_+\psi$ is an eigenvector of A_3 with eigenvalue $m+1$ unless $A_+\psi = 0$. Similarly, by Equation (10.13), $A_3(A_-\psi) = (m-1)(A_-\psi)$, so $A_-\psi$ is an eigenvector of A_3 with eigenvalue $m-1$, provided that $A_-\psi \neq 0$. (One can picture the

eigenvalues of A_3 as providing the rungs of a ladder with unit spacing between the rungs. A_+ and A_- are called "ladder operators", as they correspond to taking steps up and down the ladder.) As all basis vectors of V are eigenvectors of A^2 with the same eigenvalue, $A_+\psi$ and $A_-\psi$ are eigenvectors of A^2 with the same eigenvalue as ψ.

Let j be the *maximum* eigenvalue of A_3 in the set belonging to a particular irreducible representation $\mathbf{\Gamma}$, assume that it is non-degenerate, and let ψ_j be the corresponding eigenvector. Then $A_+\psi_j = 0$, as otherwise $(j+1)$ would be an eigenvalue of A_3. Thus $A_-A_+\psi_j = 0$ and so, from Equation (10.19), $(A^2 - A_3^2 - A_3)\psi_j = 0$. Consequently $A^2\psi_j = j(j+1)\psi_j$, so the eigenvalue of A^2 is $j(j+1)$. Thus *all* the basis vectors of this representation *must* have $j(j+1)$ as their eigenvalue with A^2.

Now consider the set of vectors $A_-\psi_j, (A_-)^2\psi_j, (A_-)^3\psi_j, \ldots$, which correspond to eigenvalues $j-1, j-2, j-3, \ldots$, with A_3. As the irreducible representation under consideration is finite-dimensional, the vectors in this sequence must become zero after a *finite* number of steps. Suppose, therefore, that k is a non-negative integer such that $(A_-)^k\psi_j \neq 0$ but $(A_-)^{k+1}\psi_j = 0$, so the *minimum* eigenvalue of A_3 is $(j-k)$. As $A_-(A_-)^k\psi_j = 0$, it follows that $A_+A_-\{(A_-)^k\psi_j\} = 0$ and consequently, by Equation (10.20), $(A^2 - A_3^2 + A_3)\{(A_-)^k\psi_j\} = 0$. But $A_3\{(A_-)^k\psi_j\} = (j-k)\{(A_-)^k\psi_j\}$ and $A^2\{(A_-)^k\psi_j\} = j(j+1)\{(A_-)^k\psi_j\}$, so this implies that

$$\{j(j+1) - (j-k)^2 + (j-k)\}\{(A_-)^k\psi_j\} = 0.$$

By assumption $\{(A_-)^k\psi_j\} \neq 0$, so $\{j(j+1) - (j-k)^2 + (j-k)\} = 0$, which gives $j = \frac{1}{2}k$. Thus the only possible values of j are $j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$. Moreover, the minimum eigenvalue of A_3 is $j - k = j - 2j = -j$. Thus the eigenvalues of A_3 are $j, j-1, j-2, \ldots, -j+1, -j$. As there are $(2j+1)$ such values, the dimension $d = 2j+1$.

Let ψ_m^j denote the simultaneous eigenvector of A^2 and A_3 with eigenvalues $j(j+1)$ and m respectively (so that ψ_j^j is the eigenvector previously denoted by ψ_j). Then, for $m = j, j-1, \ldots, -j+1$, as $A_-\psi_m^j$ is an eigenvector of A_3 with eigenvalue $(m-1)$,

$$A_-\psi_m^j = \mu_m^j\psi_{m-1}^j, \tag{10.28}$$

where μ_m^j is a complex number. As ψ_m^j and ψ_{m-1}^j are assumed to be normalized.

$$|\mu_m^j|^2 = (\mu_m^j\psi_{m-1}^j, \mu_m^j\psi_{m-1}^j) = (A_-\psi_m^j, A_-\psi_m^j) = (\psi_m^j, A_+A_-\psi_m^j)$$

(on using Equation (10.15)). However, it follows from Equation (10.20) that

$$\begin{aligned} A_+A_-\psi_m^j &= (A^2 - A_3^2 + A_3)\psi_m^j = \{j(j+1) - m^2 + m\}\psi_m^j \\ &= \{(j+m)(j-m+1)\}\psi_m^j, \end{aligned}$$

so

$$|\mu_m^j|^2 = (j+m)(j-m+1).$$

However, Equation (10.28) also implies that

$$A_+\psi^j_{m-1} = (1/\mu^j_m)A_+A_-\psi^j_m = \{|\mu^j_m|^2/\mu^j_m\}\psi^j_m.$$

Following the phase convention established by Condon and Shortley (1935), μ^j_m will be chosen to be real and positive, so that

$$\mu^j_m = \{(j+m)(j-m+1)\}^{1/2}.$$

As $\mu^j_m = 0$ for $j = -m$, Equation (10.26) follows for $m = j, j-1, \ldots, -j+l$, and $-j$. Moreover, with this convention $\{|\mu^j_m|^2/\mu^j_m\} = \mu^j_m$, so

$$A_+\psi^j_{m-1} = \mu^j_m\psi^j_m$$

for $m = j, j-1, \ldots, -j+1$. Thus

$$A_+\psi^j_m = \mu^j_{m+1}\psi^j_{m+1} = \{(j+m+1)(j-m)\}^{1/2}\psi^j_{m+1}$$

for $m = j-1, j-2, \ldots, -j$. As $\mu^j_{m+1} = 0$ for $m = j$, Equation (10.25) holds for $m = j$ as well. Clearly this representation is irreducible.

As Equation (10.5) can be rewritten as

$$\Phi(\mathbf{a})\psi^j_m = \sum_{m'=-j}^{j} D^j(\mathbf{a})_{m'm}\psi^j_{m'}$$

for all $\mathbf{a}$ of su(2) (and of $\widetilde{\mathcal{L}} = A_1$) and $m = j, j-1, \ldots, -j$, it follows that

$$D^j(\mathbf{a})_{m'm} = (\psi^j_{m'}, \Phi(\mathbf{a})\psi^j_m).$$

Consequently

$$\begin{aligned} D^j(\mathbf{a}_1)_{m'm} &= (\psi^j_{m'}, (i/2)(A_+ + A_-)\psi^j_m), \\ D^j(\mathbf{a}_2)_{m'm} &= (\psi^j_{m'}, (1/2)(A_+ - A_-)\psi^j_m), \\ D^j(\mathbf{a}_1)_{m'm} &= (\psi^j_{m'}, iA_3\psi^j_m), \end{aligned}$$

which immediately give Equations (10.27) on using Equations (10.25), (10.26) and (10.24).

This proof made use of the properties of the operator A^2, which is not itself a member of $\widetilde{\mathcal{L}}$. For proofs that do not involve A^2 see, for example, Samelson (1969) and Varadarajan (1974). It should be noted that, as the irreducible representations of su(2) are specified by j, which takes values $0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$, there is a countable infinity of such representations, in agreement with the theorem of Peter and Weyl (1927) that is stated as Theorem X of Chapter 4, Section 6.

It is interesting to examine in more detail the special cases $j = 0, \frac{1}{2}$ and 1. For $j = 0$ the irreducible representation is one-dimensional and $\mathbf{D}^0(\mathbf{a}) = [0]$

for all $\mathbf{a} \in \mathrm{su}(2)$. For $j = \frac{1}{2}$ the first and second rows are labelled by $m' = \frac{1}{2}$ and $-\frac{1}{2}$ respectively, while the first and second columns are similarly labelled by $m = \frac{1}{2}$ and $-\frac{1}{2}$. Then Equations (10.27) give

$$\mathbf{D}^{1/2}(\mathbf{a}_j) = \mathbf{a}_j,$$

the $\mathbf{a}_j$ being as in Equations (8.30), that is, $\mathbf{D}^{1/2}$ is *identical* to the defining two-dimensional representation of su(2). Similarly for $j = 1$ the rows are labelled by $m' = 1$, 0 and -1, and the columns are labelled by $m = 1$, 0 and -1, and Equations (10.27) give

$$\mathbf{D}^1(\mathbf{a}_1) = \frac{1}{2}i\begin{bmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{bmatrix}, \quad \mathbf{D}^1(\mathbf{a}_2) = \frac{1}{2}\begin{bmatrix} 0 & \sqrt{2} & 0 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 0 & -\sqrt{2} & 0 \end{bmatrix},$$

$$\mathbf{D}^1(\mathbf{a}_3) = \begin{bmatrix} i & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -i \end{bmatrix}.$$

This representation is equivalent (but not identical) to that given by the 3×3 matrices of Equations (8.12), that is, to the defining representation of so(3).

4 Representations of the Lie groups SU(2), SO(3) and O(3)

It is not difficult to show explicitly that every irreducible representation of su(2) exponentiates to give an irreducible representation of SU(2). (See, for example, Chapter 12, Section 4, of Cornwell (1984) for details.) Henceforth the $(2j + 1)$-dimensional irreducible representation of su(2) and the corresponding irreducible representation of SU(2) will *both* be denoted by the same symbol $\mathbf{D}^j$. Let $\chi^j(\mathbf{u})$ be the character of $\mathbf{D}^j$ for an element $\mathbf{u}$ of SU(2) specified by a rotation through an angle ω about an axis $\mathbf{n}$, as in Equation (10.2). As all such $\mathbf{u}$ corresponding to the same value of ω lie in the same class (irrespective of the direction of the unit vector $\mathbf{n}$), $\chi^j(\mathbf{u})$ can be calculated by taking $\mathbf{n} = (0, 0, 1)$. Then, by Equation (10.2),

$$\begin{aligned} \mathbf{u} &= \begin{bmatrix} \cos(\frac{1}{2}\omega) + i\sin(\frac{1}{2}\omega) & 0 \\ 0 & \cos(\frac{1}{2}\omega) - i\sin(\frac{1}{2}\omega) \end{bmatrix} \\ &= \begin{bmatrix} \exp(\frac{1}{2}i\omega) & 0 \\ 0 & \exp(-\frac{1}{2}i\omega) \end{bmatrix} \\ &= \exp(\omega \mathbf{a}_3), \end{aligned} \tag{10.29}$$

where $\mathbf{a}_3$ is defined in Equations (8.30). Thus $\mathbf{D}^j(\mathbf{u}) = \exp(\omega \mathbf{D}^j(\mathbf{a}_3))$, which, by Equations (10.27), is a diagonal matrix with diagonal elements $\exp(im\omega)$, m taking the values $j, j-1, \ldots, -j$. Thus

$$\chi^j(\mathbf{u}) = \sum_{m=-j}^{j} \exp(im\omega),$$

which can be rewritten as

$$\chi^j(\mathbf{u}) = \sin\{(2j+1)\omega/2\}/\sin(\omega/2). \tag{10.30}$$

Incidentally, as $\chi^1(\mathbf{u}) = 1 + 2\cos\omega$, Equation (10.4) shows that the three-dimensional representations $\mathbf{D}^1(\mathbf{u})$ and $\mathbf{R}(\mathbf{u})$ are equivalent.

Turning now to the representations of the Lie group SO(3), it is clear that the representation $\mathbf{D}^j$ of SU(2) provides a representation of SO(3) if and only if $\mathbf{D}^j(\mathbf{u}) = \mathbf{1}_{2j+1}$ for every $\mathbf{u}$ belonging to the kernel $\mathcal{K}$ of the homomorphic mapping of SU(2) onto SO(3). But $\mathcal{K}$ consists only of $\mathbf{1}_2$ and $-\mathbf{1}_2$ (see Chapter 2, Section 6), so this condition is simply that $\mathbf{D}^j(-\mathbf{1}_2) = \mathbf{1}_{2j+1}$. However, by Equation (10.2), $-\mathbf{1}_2$ corresponds to $\omega = 2\pi$ and any direction of $\mathbf{n}$. Thus, taking $\mathbf{n} = (0,0,1)$, Equation (10.29) shows that $-\mathbf{1}_2 = \exp(2\pi\mathbf{a}_3)$, so that $\mathbf{D}^j(-\mathbf{1}_2) = \exp(2\pi\mathbf{D}^j(\mathbf{a}_3))$. But Equations (10.27) indicate that this latter matrix is diagonal with diagonal entries taking the values $\exp(2\pi i m)$ with $m = j, j-1, \ldots, -j$, which are all equal to $+1$ if j is an integer, but are all equal to -1 if j is a half-integer. Consequently *the irreducible representation* $\mathbf{D}^j$ *of* su(2) *(and* so(3)*) exponentiates to give an irreducible representation* $\mathbf{D}^j$ *of* SO(3) *if and only if* j *is a non-negative integer.*

The basis functions of these representations $\mathbf{D}^j$ $(j = 0, 1, 2, \ldots)$ of SO(3) are quite easily determined. As they are basis functions of the corresponding representation $\mathbf{D}^j$ of the Lie algebra so(3) they must satisfy the equations

$$P(\mathbf{a})\psi^j_m(\mathbf{r}) = \sum_{m'=-j}^{j} D^j(\mathbf{a})_{m'm}\psi^j_{m'}(\mathbf{r})$$

for all $\mathbf{a} \in$ so(3) and $m = j, j-1, \ldots, -j$. By virtue of Equations (10.7), (10.10), (10.16), (10.23), (10.24) and (10.26), this implies that

$$-\{P(\mathbf{a}_1)^2 + P(\mathbf{a}_2)^2 + P(\mathbf{a}_3)^2\}\psi^j_m(\mathbf{r}) = j(j+1)\psi^j_m(\mathbf{r}), \tag{10.31}$$

$$-iP(\mathbf{a}_3)\psi^j_m(\mathbf{r}) = m\psi^j_m(\mathbf{r}), \tag{10.32}$$

and

$$-i\{P(\mathbf{a}_1) - iP(\mathbf{a}_2)\}\psi^j_m(\mathbf{r}) = \{(j+m)(j-m+1)\}^{1/2}\psi^j_{m-1}(\mathbf{r}). \tag{10.33}$$

Expressing Equations (8.23) in spherical polar coordinates (r, θ, ϕ) gives

$$\left.\begin{aligned} P(\mathbf{a}_1) &= -\sin\phi\,\partial/\partial\theta - \cot\theta\,\cos\phi\,\partial/\partial\phi, \\ P(\mathbf{a}_2) &= \cos\phi\,\partial/\partial\theta - \cot\theta\,\sin\phi\,\partial/\partial\phi, \\ P(\mathbf{a}_3) &= \partial/\partial\phi, \end{aligned}\right\}$$

so that Equations (10.31), (10.32) and (10.33) become

$$\{\tfrac{1}{\sin\theta}\tfrac{\partial}{\partial\theta}(\sin\theta\tfrac{\partial}{\partial\theta}) + \tfrac{1}{\sin^2\theta}\tfrac{\partial^2}{\partial\phi^2}\}\psi^j_m(\mathbf{r}) = j(j+1)\psi^j_m(\mathbf{r}), \tag{10.34}$$

$$-i\frac{\partial}{\partial\phi}\psi^j_m(\mathbf{r}) = m\psi^j_m(\mathbf{r}), \tag{10.35}$$

and

$$e^{-i\phi}\{-\tfrac{\partial}{\partial\theta}+i\cot\theta\,\tfrac{\partial}{\partial\phi}\}\psi_m^j(\mathbf{r}) \;=\{(j+m)(j-m+1)\}^{1/2}\psi_{m-1}^j(\mathbf{r}). \quad (10.36)$$

Clearly the solution of Equation (10.35) is $\psi_m^j(\mathbf{r}) = e^{im\phi}f(r,\theta)$. Substituting into Equation (10.34) gives

$$\{\tfrac{1}{\sin\theta}\tfrac{\partial}{\partial\theta}(\sin\theta\tfrac{\partial}{\partial\theta}) - \tfrac{m^2}{\sin^2\theta}\}f(r,\theta) \;= j(j+1)f(r,\theta).$$

This is the associated Legendre equation, which has as its solution

$$f(r,\theta) = P_j^m(\cos\theta)F(r),$$

where $F(r)$ is any function of r and $P_j^m(\xi)$ is the associated Legendre function, which may be defined in terms of the Legendre polynomials $P_j(\xi)$ by

$$P_j^m(\xi) = (1-\xi^2)^{m/2}(d^m/d\xi^m)P_j(\xi)$$

for $m = 0, 1, 2, \ldots, j$, and by

$$P_j^{-m}(\xi) = (-1)^m\{(j-m)!/(j+m)!\}\,P_j^m(\xi)$$

for negative values of m (see Bateman 1932, Edmonds 1957). With the "spherical harmonics" $Y_{jm}(\theta,\phi)$ defined by

$$Y_{jm}(\theta,\phi) = (-1)^m\{(2j+1)(j-m)!/4\pi(j+m)!\}^{1/2}\,e^{im\phi}\,P_j^m(\cos\theta), \quad (10.37)$$

Equations (10.34), (10.35) and (10.36) are satisfied with the ortho-normal basis functions

$$\psi_m^j(\mathbf{r}) = Y_{jm}(\theta,\phi)R(r).$$

Here $R(r)$ is any function of r alone (that is the same for all $m = j, j-1, \ldots, -j$) such that

$$\int_0^\infty |R(r)|^2 r^2\,dr = 1.$$

This depends on the ortho-normal property of the spherical harmonics:

$$\int_0^{2\pi}\int_0^{\pi} Y_{jm}^\star(\theta,\phi)\,Y_{j'm'}(\theta,\phi)\,\sin\theta\,d\theta\,d\phi = \delta_{jj'}\delta_{mm'}.$$

Clearly only the angular parts of the basis functions are significant, and this analysis shows that they are given by the spherical harmonics $Y_{jm}(\theta,\phi)$.

(In the literature there appear several different definitions of $P_j^m(\xi)$ for m negative and also different choices of the numerical factor on the right-hand side of Equation (10.37). The definitions given here are chosen so that the factor $\{(j+m)(j-m+1)\}^{1/2}$ appears on the right-hand side of Equation (10.36) in order to correspond to the phase convention of Condon and Shortley (1935). See Edmonds (1957) for a thorough discussion of these points.)

Finally, consider the group of *all* rotations in $\mathbb{R}^3$, both proper *and* improper, which is isomorphic to O(3). As noted in Example I of Chapter 2, Section 7, O(3) is isomorphic to the direct product of SO(3) with the group of order 2 consisting of matrices $\mathbf{1}_3$ and $-\mathbf{1}_3$. As this latter group has only two irreducible representations, both one-dimensional, which may be labelled $\mathbf{\Gamma}^1$ and $\mathbf{\Gamma}^{-1}$ in such a way that

$$\mathbf{\Gamma}^1(\mathbf{1}_3) = [1],\ \mathbf{\Gamma}^1(-\mathbf{1}_3) = [1],\ \mathbf{\Gamma}^{-1}(\mathbf{1}_3) = [1],\ \mathbf{\Gamma}^{-1}(-\mathbf{1}_3) = [-1],$$

Theorem I of Chapter 5, Section 5, shows that for $j = 0, 1, 2, \ldots$ the group O(3) has *two* inequivalent irreducible representations of dimension $(2j+1)$, which may be denoted by $\mathbf{\Gamma}^{p,j}$ ($p = 1$ or -1) and which are defined by

$$\left.\begin{array}{rclrcl} \mathbf{\Gamma}^{1,j}(\mathbf{R}) & = & \mathbf{D}^j(\mathbf{R}), & \mathbf{\Gamma}^{1,j}(-\mathbf{R}) & = & \mathbf{D}^j(\mathbf{R}), \\ \mathbf{\Gamma}^{-1,j}(\mathbf{R}) & = & \mathbf{D}^j(\mathbf{R}), & \mathbf{\Gamma}^{-1,j}(-\mathbf{R}) & = & -\mathbf{D}^j(\mathbf{R}), \end{array}\right\}$$

for each $\mathbf{R} \in \mathrm{SO}(3)$, $\mathbf{D}^j$ being the irreducible representation of SO(3) discussed above. The quantity p may be called "parity".

As for the spatial inversion operator I, as $P(I)Y_{jm}(\theta,\phi) = (-1)^j Y_{jm}(\theta,\phi)$, the basis functions $Y_{jm}(\theta,\phi)F(r)$ of $\mathbf{D}^j$ are basis functions of $\mathbf{\Gamma}^{p,j}$ *only when* $p = (-1)^j$. Consequently the irreducible representations $\mathbf{\Gamma}^{p,j}$ of O(3) with $p = -(-1)^j$ *possess no basis functions.*

This does *not* mean that the irreducible representations $\mathbf{\Gamma}^{p,j}$ of O(3) with $p = -(-1)^j$ have no physical significance, for it is possible to have irreducible tensor operators transforming according to such a representation. The most important example where this is so is that of the orbital angular momentum operators L_x, L_y and L_z of Equations (8.26). Indeed, Equations (8.26) and (9.34) show that L_x, L_y and L_z transform as irreducible tensor operators of the three-dimensional adjoint representation of SO(3), which is easily shown to be equivalent to $\mathbf{D}^1$. Moreover, for the spatial inversion operator I, Equations (5.29) show that $P(I)\partial/\partial x P(I)^{-1} = -\partial/\partial x$, $P(I)\partial/\partial y P(I)^{-1} = -\partial/\partial y$, and $P(I)\partial/\partial z P(I)^{-1} = -\partial/\partial z$, while Example IV of Chapter 5, Section 3, shows that $P(I)xP(I)^{-1} = -x$, $P(I)yP(I)^{-1} = -y$, and $P(I)zP(I)^{-1} = -z$. Consequently Equations (8.23) and (8.26) imply that $P(I)L_xP(I)^{-1} = L_x$, $P(I)L_yP(I)^{-1} = L_y$, and $P(I)L_zP(I)^{-1} = L_z$. Thus L_x, L_y and L_z transform as irreducible tensor operators of a representation of O(3) that is equivalent to $\mathbf{\Gamma}^{1,1}$. In fact, as $[P(\mathbf{a}_3), L_z] = 0$, the operator L_z transforms as the row labelled by $m = 0$ of $\mathbf{\Gamma}^{1,1}$.

5 Direct products of irreducible representations and the Clebsch-Gordan coefficients

The analysis of Chapter 9, Section 4, shows that it is merely a matter of convenience whether the Clebsch-Gordan series and Clebsch-Gordan coefficients are derived in terms of the Lie algebra su(2) (or so(3)) or the Lie group SU(2) (or SO(3)). In this particular situation, the Clebsch-Gordan series is found most

directly by a group theoretical argument, but the Clebsch-Gordan coefficients are most easily deduced by algebraic considerations. (In other cases it is usually much easier to use the Lie algebraic arguments for both Clebsch-Gordan series and coefficients.)

Theorem I The Clebsch-Gordan series for the direct product of two irreducible representations $\mathbf{D}^{j_1}$ and $\mathbf{D}^{j_2}$ of SU(2) is

$$\mathbf{D}^{j_1} \otimes \mathbf{D}^{j_2} \approx \mathbf{D}^{j_1+j_2} \oplus \mathbf{D}^{j_1+j_2-1} \oplus \ldots \oplus \mathbf{D}^{|j_1-j_2|+1} \oplus \mathbf{D}^{|j_1-j_2|}, \qquad (10.38)$$

where $\mathbf{D}^j$ appears on the right-hand side once and only once for j taking values from $(j_1 + j_2)$ down to $|j_1 - j_2|$ in integral steps. (This is also the Clebsch-Gordan series for su(2) and so(3), and for SO(3) provided j_1 and j_2 take integral values.)

Proof By Equations (5.14) and (10.30), the character $\chi^{j_1 \otimes j_2}(\mathbf{u})$ of $\mathbf{D}^{j_1} \otimes \mathbf{D}^{j_2}$ for an element $\mathbf{u}$ of SU(2) specified, as in Equation (10.2), by a rotation through an angle ω about an axis in the direction $\mathbf{n}$ is

$$\chi^{j_1 \otimes j_2}(\mathbf{u}) = [\sin\{(2j_1 + 1)\omega/2\} \sin\{(2j_2 + 1)\omega/2\}]/\sin^2(\omega/2).$$

But

$$\begin{aligned}
\sum_{j=|j_1-j_2|}^{j_1+j_2} \chi^j(\mathbf{u}) &= \mathrm{Im}[\textstyle\sum_{j=|j_1-j_2|}^{j_1+j_2} \exp\{(2j + 1)\omega/2\}]/\sin(\omega/2) \\
&= \mathrm{Im}[i\{\exp(i|j_1 - j_2|\omega) - \exp(i(j_1 + j_2 + 1)\omega)\}]/\sin^2(\omega/2) \\
&= [\cos\{(j_1 - j_2)\omega\} - \cos\{(j_1 + j_2 + 1)\omega\}]/\sin^2(\omega/2) \\
&= \chi^{j_1 \otimes j_2}(\mathbf{u})
\end{aligned}$$

for all $\mathbf{u} \in$ SU(2), from which Equation (10.38) follows immediately.

As Equation (10.38) implies that

$$n^j_{j_1,j_2} = \begin{cases} 1, & \text{if } j = j_1 + j_2, j_1 + j_2 - 1, \ldots, |j_1 - j_2|, \\ 0, & \text{for all other values of } j, \end{cases} \qquad (10.39)$$

the index α that appeared in the general expressions in Equations (5.35), (5.36), (9.28) and (9.29) is redundant and can, therefore, be omitted from Equations (5.36) and (9.29). At the same time, the Clebsch-Gordan coefficients will be rewritten in a slightly different notation that is widely used in the literature on angular momentum, as follows:

$$\left(\begin{array}{cc|cc} j_1 & j_2 & j, & 1 \\ m_1 & m_2 & m & \end{array} \right) = (j_1, m_1, j_2, m_2 \mid j_1, j_2, j, m)$$

(Edmonds 1957). In this context Equations (5.35) and (9.28) become

$$\theta^j_m = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} (j_1, m_1, j_2, m_2 \mid j_1, j_2, j, m)\, \psi^{j_1}_{m_1} \otimes \psi^{j_2}_{m_2}, \qquad (10.40)$$

where θ^j_m transforms as the row labelled by m $(= -j, -j+1, \ldots, j)$ of the irreducible representation $\mathbf{D}^j$ appearing in $\mathbf{D}^{j_1} \otimes \mathbf{D}^{j_2}$.

Of course the double appearance of j_1 and j_2 in these coefficients is unnecessary, but is accepted because of the natural way in which this notation is suggested in the theory of addition of angular momentum (cf. Chapter 12, Section 5, of Cornwell (1984)). These quantities are sometimes referred to alternatively as "vector-coupling" or "Wigner" coefficients. The book by Edmonds (1957) contains a description of the various other notations that have been used for these coefficients.

The Lie algebraic considerations that lead to explicit expressions for the Clebsch-Gordan coefficients will be omitted here (but a detailed introductory account appears, for example, in Chapter 12, Section 5, of Cornwell (1984)). Wigner (1959), Racah (1942), Schwinger (1952) and Edmonds (1957) have used these ideas to produce general formulae for the Clebsch-Gordan coefficients, the expression derived by Edmonds (1957) being

$$\begin{aligned}
&(j_1, m_1, j_2, m_2 \mid j_1, j_2, j, m) \\
&= \{(2j+1)(j_1+j_2-j)!(j_1-j_2+j)!(-j_1+j_2+j)!/(j_1+j_2+j+1)!\}^{1/2} \\
&\quad \times \{(j_1+m_1)!(j_1-m_1)!(j_2+m_2)!(j_2-m_2)!(j+m)!(j-m)!\}^{1/2} \\
&\quad \times \sum_z (-1)^z \{z!(j_1+j_2-j-z)!(j_1-m_1-z)!(j_2+m_2-z)! \\
&\quad \times (j-j_2+m_1+z)!(j-j_1-m_2+z)!\}^{-1} \delta_{m_1+m_2,m}. \qquad (10.41)
\end{aligned}$$

(Here the sum is over those non-negative integer values of z for which all of the factors $(j_1+j_2-j-z)!$, $(j_1-m_1-z)!$, $(j_2+m_2-z)!$, $(j-j_2+m_1+z)!$ and $(j-j_1-m_2+z)!$ are non-negative.) Simpler formulae may be obtained for special cases, and are discussed in the references just given and in the books by Rose (1957) and Biedenharn and Louck (1979a,b). These works also contain explicit tabulations of Clebsch-Gordan coefficients, further extensive tables being given by Condon and Shortley (1935) and Cohen (1974). See also Butler (1981). All these Clebsch-Gordan coefficients may be taken to be *real*.

It is easy to extend these results to the group O(3). With notation for irreducible representations of O(3) introduced in Section 4, the Clebsch-Gordan series for O(3) is

$$\mathbf{\Gamma}^{p_1,j_1} \otimes \mathbf{\Gamma}^{p_2,j_2} \approx \mathbf{\Gamma}^{p_1p_2,j_1+j_2} \oplus \mathbf{\Gamma}^{p_1p_2,j_1+j_2-1} \oplus \ldots \oplus \mathbf{\Gamma}^{p_1p_2,|j_1-j_2|} \qquad (10.42)$$

(p_1 and p_2 taking the values 1 and -1). Note that the parity p of *every* irreducible representation $\mathbf{\Gamma}^{p,j}$ in the Clebsch-Gordan series is the *product* of the parities p_1 and p_2 of the irreducible representations in the direct product. (This follows because with $\Phi^{p,j}(I)\psi^{p,j}_m = p\psi^{p,j}_m$, Equation (5.33) gives $\Phi(I)\{\psi^{p_1,j_1}_{m_1} \otimes \psi^{p_2,j_2}_{m_2}\} = (p_1p_2)\{\psi^{p_1,j_1}_{m_1} \otimes \psi^{p_2,j_2}_{m_2}\}$, the rest of the content of Equation (10.42) being determined by the corresponding series of Equation (10.38) for the subgroup SO(3)). It is obvious that for $p = p_1p_2$ the Clebsch-

Gordan coefficients of O(3) are given by

$$\left(\begin{array}{cc|cc} p_1, j_1 & p_2, j_2 & p, j, & 1 \\ m_1 & m_2 & m & \end{array} \right) = (j_1, m_1, j_2, m_2 \,|\, j_1, j_2, j, m), \qquad (10.43)$$

where $(j_1, m_1, j_2, m_2 | j_1, j_2, j, m)$ are the Clebsch-Gordan coefficients of SO(3) described above.

6 Applications to atomic physics

The ideas developed in the previous sections will now be applied to the "one-electron" theory of atomic structure, that is, to the theory in which each electron of the atom is assumed to move in the average field of all the other electrons, the resulting potential energy being assumed to be spherically symmetrical. Although some important results will be derived in this section, the discussion is primarily intended to indicate the sort of conclusions that can be obtained. For more detailed accounts based on more elaborate models of atomic structure, the reader is referred to the monographs of Condon and Odabasi (1980), Wigner (1959) and Wybourne (1970).

In this section the dynamical effects of the spin of the electron will be neglected. (For an introductory account in which they are included, see Chapter 12, Section 6, of Cornwell (1984)). With this assumption the wave function of the electron is a scalar function and the theory introduced in Chapter 1, Section 3, applies. In this situation the group of the Schrödinger equation is the group of all rotations in $\mathbb{R}^3$. The theory of Chapter 1, Section 4 then shows that the eigenfunctions of the time-independent Schrödinger equation are basis functions of the irreducible representations of this group. These were deduced at the end of Section 4 above.

Before proceeding further it is convenient to make a small change in notation to give that used in the physics literature. As noted in Equation (8.26), the operators $P(\mathbf{a}_1)$, $P(\mathbf{a}_2)$ and $P(\mathbf{a}_3)$ are merely the orbital angular momentum operators L_x, L_y and L_z multiplied by a factor $(i/\hbar)$. Consequently the basis functions $\psi_m^j(\mathbf{r})$ of Section 4 are, by Equations (10.31) and 10.32), eigenfunctions of the "total" angular momentum operator L^2 (defined by $L^2 = L_x^2 + L_y^2 + L_z^2$) and L_z with eigenvalues $\hbar^2 j(j+1)$ and $\hbar m$ respectively. This first eigenvalue is normally denoted by $\hbar^2 l(l+1)$ (with $l = 0, 1, 2, \ldots$), so for the rest of the discussion of representations of SO(3) and O(3), l will be used in place of j. The integer l is called the "azimuthal" or "orbital angular momentum quantum number", and the integer m is known as the "magnetic quantum number" because of its role in the Zeeman effect (which will be described shortly). With this change the eigenfunctions of the time-independent Schrödinger equation are labelled by l and m (with $l = 0, 1, 2, \ldots$, and $m = l, l-1, \ldots, -l$), together with another quantum number, usually denoted by n and called the "total quantum number", associated with the solution of the radial part of the time-independent Schrödinger equation. Let $\psi_{nm}^l(\mathbf{r}) = R_{nl}(r) Y_{lm}(\theta, \phi)$ be such an eigenfunction. (It is common

to call states corresponding to $l = 0, 1, 2, 3, \ldots$, respectively s-states, p-states, d-states, f-states and so on.)

The first application will be to the selection rules for optical transitions within the "dipole" approximation described in Chapter 6, Section 2. In the present case $\mathcal{G}_0$ (the invariance group of the unperturbed Hamiltonian) is the group of *all* rotations in $\mathbb{R}^3$. Transitions from an initial state $\phi_i(\mathbf{r})$ to a final state $\phi_f(\mathbf{r})$ (both assumed to be basis functions of some irreducible representations of $\mathcal{G}_0$) are forbidden if $(\phi_f, Q\phi_f) = 0$, where $Q = \mathbf{A}_0.\mathbf{grad}$ for absorption or induced emission in an electromagnetic field whose polarization is specified by the constant vector $\mathbf{A}_0$ and where $Q = \mathbf{n}.\mathbf{grad}$ for spontaneous emission polarized in the direction of the unit vector $\mathbf{n}$.

Equations (5.29) show that the components of the operator **grad** transform as irreducible tensor operators of the representation of O(3) defined by $\mathbf{\Gamma}(\mathbf{R}) = \mathbf{R}$ for all $\mathbf{R} \in \mathrm{O}(3)$. This is equivalent to the irreducible representation $\mathbf{\Gamma}^{-1,1}$ of O(3) in the notation introduced in Section 4. Indeed, Equations (8.23) show that

$$\left.\begin{array}{lll} [P(\mathbf{a}_1), \frac{\partial}{\partial x}] = 0, & [P(\mathbf{a}_1), \frac{\partial}{\partial y}] = -\frac{\partial}{\partial z}, & [P(\mathbf{a}_1), \frac{\partial}{\partial z}] = \frac{\partial}{\partial y}, \\ [P(\mathbf{a}_2), \frac{\partial}{\partial x}] = \frac{\partial}{\partial z}, & [P(\mathbf{a}_2), \frac{\partial}{\partial y}] = 0, & [P(\mathbf{a}_2), \frac{\partial}{\partial z}] = -\frac{\partial}{\partial x}, \\ [P(\mathbf{a}_3), \frac{\partial}{\partial x}] = -\frac{\partial}{\partial y}, & [P(\mathbf{a}_3), \frac{\partial}{\partial y}] = \frac{\partial}{\partial x}, & [P(\mathbf{a}_3), \frac{\partial}{\partial z}] = 0. \end{array}\right\} \tag{10.44}$$

Taken with Equation (9.34) and the matrices for $\mathbf{D}^1$ given at the end of Section 3, Equations (10.44) imply that $-(1/\sqrt{2})(\partial/\partial x + i\partial/\partial y)$, $\partial/\partial z$ and $(1/\sqrt{2})(\partial/\partial x - i\partial/\partial y)$ transform as irreducible tensor operators belonging to the $m = 1$, $m = 0$ and $m = -1$ rows of the irreducible representation $\mathbf{D}^1$ of SO(3) and hence then transform according to the same rows of the representation $\mathbf{\Gamma}^{-1,1}$ of O(3).

Now suppose that the initial state eigenfunction $\phi_i(\mathbf{r})$ is the basis function $\psi^l_{nm}(\mathbf{r})$ belonging to the row labelled by m of the irreducible representation $\mathbf{\Gamma}^{p,l}$ of O(3), where $p = (-1)^l$. Suppose first that $l \geq 1$. Then, by Equation (10.42) (with $p_1 = p(-1)^l$, $j_1 = l$, $p_2 = -1$, $j_2 = 1$),

$$\mathbf{\Gamma}^{p,l} \otimes \mathbf{\Gamma}^{-1,1} \approx \mathbf{\Gamma}^{-p,l+1} \oplus \mathbf{\Gamma}^{-p,l} \oplus \mathbf{\Gamma}^{-p,l-1}, \tag{10.45}$$

so that the only possible final state eigenfunctions $\phi_f(\mathbf{r})$ are basis functions of the irreducible representations on the right hand side of Equation (10.45). However, there are no basis functions transforming as $\mathbf{\Gamma}^{-p,l}$ (as with $-p = -(-1)^l$ the parity has the "wrong" value (see Section 4), so that $\phi_f(\mathbf{r})$ can only be a basis function of $\mathbf{\Gamma}^{-p,l+1}$ or $\mathbf{\Gamma}^{-p,l-1}$. That is, assuming $l \geq 1$, if $\phi_f(\mathbf{r}) = \psi^{l'}_{n'm'}(\mathbf{r})$, then

$$l' = l + 1 \text{ or } l - 1. \tag{10.46}$$

Similarly, if $l = 0$, Equation (10.42) gives

$$\mathbf{\Gamma}^{1,0} \otimes \mathbf{\Gamma}^{-1,1} \approx \mathbf{\Gamma}^{-1,1}, \tag{10.47}$$

so that $\phi_f(\mathbf{r})$ can only transform as $\mathbf{\Gamma}^{-1,1}$. That is, for $l = 0$, l' can only be given by

$$l' = l + 1. \tag{10.48}$$

Further selection rules exist for polarized radiation. For $\mathbf{A}_0$ or $\mathbf{n}$ in the z-direction, $Q = \partial/\partial z$, which transforms as the $m = 0$ row of $\mathbf{\Gamma}^{-1,1}$. Then the Wigner-Eckart Theorem, taken with Equations (10.41) and (10.43), implies that

$$m' = m. \tag{10.49}$$

Similarly, for $\mathbf{A}_0$ or $\mathbf{n}$ in the x- or y-direction, Q transforms as a combination of irreducible tensor operators belonging to the $m = 1$ and $m = -1$ rows of $\mathbf{\Gamma}^{-1,1}$, implying that

$$m' = (m + 1) \text{ or } (m - 1). \tag{10.50}$$

The selection rules of Equations (10.49) and (10.50) become observable if a small magnetic field $\mathbf{H} = (H_x, H_y, H_z)$ is applied to the system. The resulting theory provides an example of the general technique described in Chapter 6, Section 3. The perturbing term H' in the Hamiltonian H is

$$H' = -(e/2\mu c)\{H_x L_x + H_y L_y + H_z L_z\}, \tag{10.51}$$

L_x, L_y and L_z being the orbital angular momentum operators and e and μ the charge and mass of the electron (Schiff 1968). Without loss of generality it may be assumed that the coordinate axes are chosen so that Oz is in the direction of $\mathbf{H}$, so that

$$H' = -(e/2\mu c)H_z L_z. \tag{10.52}$$

The analysis at the end of Section 4 shows that H' is an irreducible tensor operator transforming as the $m = 0$ row of the irreducible representation $\mathbf{\Gamma}^{1,1}$ of the invariance group $\mathcal{G}_0 = \mathrm{O}(3)$ of the unperturbed Hamiltonian

$$H_0 = -(\hbar^2/2\mu)\nabla^2 + V(r).$$

Consequently the invariance group $\mathcal{G}$ of the perturbed Hamiltonian $H(= H_0 + H')$ is the direct product of the group SO(2) of all proper rotations about Oz with the group $\{E, I\}$.

Consider the unperturbed energy level ϵ_0 corresponding to the eigenfunction $\psi^l_{nm}(\mathbf{r})$ that is a basis function of the irreducible representation $\mathbf{\Gamma}^{p,l}$ of O(3) (with $p = (-1)^l$). This has degeneracy $2(2l + 1)$ (the factor 2 being due to the electron's spin). However, the irreducible representations of SO(2) are all one-dimensional and are given by

$$\mathbf{\Gamma}^m \left(\begin{bmatrix} \cos\omega & \sin\omega & 0 \\ -\sin\omega & \cos\omega & 0 \\ 0 & 0 & 1 \end{bmatrix} \right) = [e^{im\omega}] \tag{10.53}$$

for all integral values of m, both positive and negative (as SO(2) is isomorphic to U(1)), and these are the irreducible representations of U(1). As the character χ^l of the irreducible representation $\mathbf{D}^l$ of SO(3) for this rotation is

$\sum_{m=-l}^{l} \exp(im\omega)$ (see Section 4), it follows immediately that the reduction of $\mathbf{D}^l$ of SO(3) into irreducible representations of SO(2) is simply

$$\mathbf{D}^l \approx \mathbf{\Gamma}^l \oplus \mathbf{\Gamma}^{l-1} \oplus \ldots \oplus \mathbf{\Gamma}^{-l+1} \oplus \mathbf{\Gamma}^{-l}. \tag{10.54}$$

In fact, with $\mathbf{D}^l$ specified as in Sections 3 and 4, $\mathbf{D}^l$ is actually the direct sum of these irreducible representations of SO(2), *no* similarity transformation being needed to execute the reduction. (That is, the matrix $\mathbf{S}$ of Chapter 6, Section 3, is the identity matrix $\mathbf{1}_{2l+1}$.) One therefore expects for $l \geq 1$ that the unperturbed energy level ϵ_0 will be split into $(2l+1)$ different energy levels by the magnetic field (each having a two-fold degeneracy because of the electron's spin).

This prediction is easily confirmed. For $l \geq 1$ Equation (10.42) gives

$$\mathbf{\Gamma}^{1,1} \otimes \mathbf{\Gamma}^{p,l} \approx \mathbf{\Gamma}^{p,l+1} \oplus \mathbf{\Gamma}^{p,l} \oplus \mathbf{\Gamma}^{p,l-1}, \tag{10.55}$$

the appearance of $\mathbf{\Gamma}^{p,l}$ on the right-hand side of Equation (10.55) indicating that the energy levels are perturbed to first order. The perturbed levels are the eigenvalues of the $(2l+1) \times (2l+1)$ matrix $\mathbf{A}$ whose elements are given (in the present notation) by

$$A_{m'm} = \epsilon_0 \delta_{m'm} + (\psi^l_{nm'}, H'\psi^l_{nm})$$

for $m, m' = l, l-1, \ldots, -l+1, -l$ (cf. Equation (6.19)), ϵ_0 being the unperturbed energy eigenvalue. However, by Equations (10.52) and (8.26), $H' = -(e\hbar H_z/2\mu ci)P(\mathbf{a}_3)$, so that, by Equation (10.24)

$$H'\psi^l_{nm}(\mathbf{r}) = -(e\hbar H_z/2\mu c)m\psi^l_{nm}(\mathbf{r}).$$

Thus

$$A_{m'm} = \delta_{m'm}\{\epsilon_0 - (e\hbar H_z/2\mu c)m\}.$$

Consequently the perturbed energy eigenvalues are

$$\epsilon_0 - (e\hbar H_z/2\mu c)m \tag{10.56}$$

for $m = l, l-1, \ldots, -l+1, -l$. (This analysis shows that because of the simple form of H' it is not necessary in this case to invoke the Wigner-Eckart Theorem to deduce the quantities $(\psi^l_{nm'}, H'\psi^l_{nm})$).

Chapter 11

The Structure of Semi-simple Lie Algebras

1 An outline of the presentation

The theory of semi-simple Lie algebras is worth studying in detail, not only because of its elegance and completeness but also because of its considerable physical applications, particularly in elementary particle theory.

The present chapter is devoted to the study of the *structure* of semi-simple Lie algebras. Section 2 gives the definitions of simple and semi-simple Lie algebras and contains a very useful criterion of Cartan. The process of "complexification", that is, of going from a real Lie algebra to a complex Lie algebra, is then investigated in Section 3, with particular emphasis on the semi-simple case. Most of the rest of the chapter is devoted to the structure of the semi-simple *complex* Lie algebras, for which the complete classification is presented. The semi-simple *real* Lie algebras are the subject of the last section of this chapter. Chapter 12 contains the basic ideas of representation theory of semi-simple Lie algebras and Lie groups together with examples.

Appendix D contains some detailed information on the properties of simple Lie algebras.

2 The Killing form and Cartan's criterion

The developments of this section apply equally to real and complex Lie algebras (except where explicitly stated otherwise). The relationship between real and complex Lie algebras will be examined in the next section, particularly for the simple and semi-simple cases.

Definition *Simple Lie algebra*
A Lie algebra $\mathcal{L}$ is said to be "simple" if it is not Abelian and does not possess a proper invariant Lie subalgebra.

The definitions of the terms "proper" and "invariant" were given in Chapter 9, Section 2, the term "Abelian" having been introduced in Chapter 8, Section 4. Here (as throughout this book) the convention applies that every Lie algebra and subalgebra has dimension greater than zero.

Definition *Semi-simple Lie algebra*
A Lie algebra $\mathcal{L}$ is said to be "semi-simple" if it does not possess an Abelian invariant subalgebra.

The definitions imply that if $\mathcal{L}$ is simple then $\mathcal{L}$ is certainly semi-simple. However, the converse is not true, for if $\mathcal{L} = \mathrm{su}(2) \oplus \mathrm{su}(3)$ then $\mathcal{L}$ is semi-simple, but $\mathcal{L}$ is not simple because it possesses invariant subalgebras isomorphic to su(2) and su(3).

If $\mathcal{L}$ is Abelian then $\mathcal{L}$ is neither simple nor semi-simple. (Such an algebra is barred explicitly from being simple, and is implicitly prevented from being semi-simple because it is an Abelian invariant subalgebra of itself.) As all one-dimensional Lie algebras are Abelian, simple and semi-simple Lie algebras must have dimension greater than one.

Definition *Simple linear Lie group*
A linear Lie group $\mathcal{G}$ is said to be "simple" if and only if its real Lie algebra $\mathcal{L}$ is simple.

Definition *Semi-simple linear Lie group*
A linear Lie group $\mathcal{G}$ is said to be "semi-simple" if and only if its real Lie algebra $\mathcal{L}$ is semi-simple

Thus a simple linear Lie group is semi-simple, but the converse is not necessarily true. If $\mathcal{G}$ is Abelian or possesses a proper Abelian invariant Lie subgroup, then $\mathcal{G}$ is not semi-simple (see Theorem I of Chapter 9, Section 2). The treatment of examples will be deferred until the end of this section, when Cartan's criterion will have been introduced.

The "Killing form", which will now be defined, provides not only a very convenient criterion for distinguishing semi-simple Lie algebras but also plays an important part in the analysis of the structure of such algebras.

Definition *Killing form*
The "Killing form" $B(a, b)$ corresponding to any two elements a and b of a Lie algebra $\mathcal{L}$ is defined by

$$B(a, b) = \mathrm{tr}\,\{\mathbf{ad}(a)\mathbf{ad}(b)\}, \tag{11.1}$$

where $\mathbf{ad}(a)$ denotes the matrix representing $a \in \mathcal{L}$ in the *adjoint* representation of $\mathcal{L}$ (as defined in Chapter 9, Section 5) and tr denotes the trace of the matrix product (see Appendix A, Section 1).

If $\mathcal{L}$ is a *real* Lie algebra, all the matrix elements of $\mathbf{ad}(a)$ are real for each

$a \in \mathcal{L}$, so that in this case $B(a,b)$ is *real* for all $a, b \in \mathcal{L}$. This will not be so when $\mathcal{L}$ is complex.

Example I *The Killing form of* $\mathcal{L} = \mathrm{su}(2)$
With the commutation relations (Equations (8.31)) of $\mathcal{L} = \mathrm{su}(2)$, Equation (9.36) implies that

$$\mathbf{ad}(\mathbf{a}_1) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}, \quad \mathbf{ad}(\mathbf{a}_2) = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix},$$

$$\mathbf{ad}(\mathbf{a}_3) = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

from which it follows by Equation (11.1) that

$$B(\mathbf{a}_p, \mathbf{a}_q) = -2\delta_{pq}$$

for $p, q = 1, 2, 3$.

Example II *The Killing form of* $\mathcal{L} = \mathrm{sl}(2, \mathbb{R})$
As noted in Table 8.1 of Chapter 8, Section 5, $\mathcal{L} = \mathrm{sl}(2, \mathbb{R})$ is the real Lie algebra of traceless real 2×2 matrices. A convenient choice of basis is

$$\mathbf{b}_1 = \frac{1}{2}\begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}, \quad \mathbf{b}_2 = \frac{1}{2}\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad \mathbf{b}_3 = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \tag{11.2}$$

giving the basic commutation relations

$$[\mathbf{b}_1, \mathbf{b}_2] = \mathbf{b}_3, \ [\mathbf{b}_2, \mathbf{b}_3] = \mathbf{b}_1, \ [\mathbf{b}_3, \mathbf{b}_1] = -\mathbf{b}_2.$$

(It will be noted that the first two of these differ by a sign from the corresponding relations for su(2) (Equations (8.31)).) Thus, by Equation (9.36),

$$\mathbf{ad}(\mathbf{b}_1) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \quad \mathbf{ad}(\mathbf{b}_2) = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix},$$

$$\mathbf{ad}(\mathbf{b}_3) = \begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

and consequently

$$B(\mathbf{b}_1, \mathbf{b}_1) = 2, \ B(\mathbf{b}_2, \mathbf{b}_2) = -2, \ B(\mathbf{b}_3, \mathbf{b}_3) = 2,$$

and, for $p \neq q$, $(p, q = 1, 2, 3)$,

$$B(\mathbf{b}_p, \mathbf{b}_q) = 0.$$

The main properties of the Killing form are summarized in the following theorem:

Theorem I The Killing form is a symmetric bilinear form. (See Appendix B, Section 5). That is

(a) $B(a,b) = B(b,a)$, for all $a, b \in \mathcal{L}$;

(b) $B(\alpha a, \beta b) = \alpha\beta B(a,b)$, for all $a, b \in \mathcal{L}$, α and β being any pair of real numbers if $\mathcal{L}$ is real or any pair of complex numbers if $\mathcal{L}$ is complex;

(c) $B(a, b+c) = B(a,b) + B(a,c)$, for all $a, b, c \in \mathcal{L}$.

Also

(d) if ψ is any automorphism of $\mathcal{L}$, $B(\psi(a), \psi(b)) = B(a,b)$ for all $a, b \in \mathcal{L}$;

(e) $B([a,b],c) = B(a,[b,c])$, for all $a, b, c \in \mathcal{L}$;

(f) if $\mathcal{L}'$ is an invariant subalgebra of $\mathcal{L}$, and $B_{\mathcal{L}'}$ denotes the Killing form of $\mathcal{L}'$ considered as a Lie algebra in its own right, then $B(a,b) = B_{\mathcal{L}'}(a,b)$ for all $a, b \in \mathcal{L}'$.

Proof See, for example, Appendix E, Section 6, of Cornwell (1984).

The key to the whole theory of semi-simple Lie algebras is provided by "Cartan's criterion for semi-simplicity", which is as follows:

Theorem II A Lie algebra $\mathcal{L}$ is *semi-simple* if and only its Killing form is *non-degenerate*. That is, $\mathcal{L}$ is semi-simple if and only if $\det \mathbf{B} \neq 0$, where $\mathbf{B}$ is the $n \times n$ matrix whose elements are defined by $B_{pq} = B(\mathbf{a}_p, \mathbf{a}_q)$ (for $p, q = 1, 2, \ldots, n$), $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n$ being a basis for $\mathcal{L}$.

(The account of non-degenerate bilinear forms given in Appendix B, Section 5, shows the equivalence of the two conditions appearing in the statement of the theorem.)

Proof See, for example, Appendix E, Section 6, of Cornwell (1984).

The following theorem shows that the study of *semi-simple* algebras reduces to the study of *simple* Lie algebras.

Theorem III Every semi-simple Lie algebra is either simple or is the direct sum of a set of simple Lie algebras. That is, if $\mathcal{L}$ is a semi-simple Lie algebra then there exists a set of invariant subalgebras $\mathcal{L}_1, \mathcal{L}_2, \ldots, \mathcal{L}_k$ $(k \geq 1)$ which are simple, such that

$$\mathcal{L} = \mathcal{L}_1 \oplus \mathcal{L}_2 \oplus \ldots \oplus \mathcal{L}_k. \tag{11.3}$$

Moreover, this decomposition is unique.

Proof See, for example, Appendix E, Section 6, of Cornwell (1984).

A further reason for studying a semi-simple Lie algebra by means of its adjoint representation is provided by the following theorem.

Theorem IV If $\mathcal{L}$ is semi-simple then its adjoint representation **ad** is *faithful.*

Proof Suppose that **ad** is not faithful, so that there exist two elements $a, b \in \mathcal{L}$ such that $\mathbf{ad}(a) = \mathbf{ad}(b)$ but $a \neq b$. Then $\mathbf{ad}(a - b) = 0$. Hence, for any $c \in \mathcal{L}$, $\mathbf{ad}(a - b)\mathbf{ad}(c) = 0$, so that $B(a - b, c) = 0$. Thus the Killing form is degenerate, and hence $\mathcal{L}$ cannot be semi-simple.

The adjoint representation has a further important property:

Theorem V If $\mathcal{L}$ is simple then its adjoint representation is *irreducible.*

Proof The carrier space V of the adjoint representation of $\mathcal{L}$ can be identified with $\mathcal{L}$ itself, with the operator $ad(a)$ $(a \in \mathcal{L})$ acting in $\mathcal{L}$ defined for all $b \in \mathcal{L}$ by $ad(a)\, b = [a, b]$ (see Chapter 9, Section 5). If **ad** is reducible there must exist a non-trivial subspace V' of V such that $V' \neq V$ and $ad(a)b' \in V'$ for all $a \in \mathcal{L}$ and $b' \in V'$. That is $[a, b'] \in V'$ for all $a \in \mathcal{L}$ and $b' \in V'$. Thus V' is a proper invariant subspace of $\mathcal{L}$, which is impossible if $\mathcal{L}$ is simple. Thus **ad** must be irreducible.

Example III *The groups* SU(N), $N \geq 2$

SU(N) is simple for all $N \geq 2$. For the case $N = 2$, this is a straightforward consequence of results already obtained. In fact Example I above shows that $\det \mathbf{B} = (-2)^3 = -8$ $(\neq 0)$, so that Cartan's criterion implies that su(2) is semi-simple. But su(2) must be simple, as otherwise su(2) has a decomposition of the form of Equation (11.3) with at least two members. This is not possible, as the dimension of su(2) is 3, while the dimension of every simple Lie algebra is greater than or equal to 2.

For $N \neq 3$ the "simplicity" of su(N) can be demonstrated by identifying su(N) with one of a set of simple Lie algebras. (See, for example, Appendix G, Section 1, of Cornwell (1984).)

Example IV *The groups* SO(N), $N \geq 2$

(i) SO(2) is Abelian and therefore not simple.

(ii) SO(3) is simple, as so(3) is isomorphic to su(2) (see Example III of Chapter 9, Section 3) which, as shown in Example III above, is simple.

(iii) SO(4) is semi-simple but not simple, for it can be shown that SO(4) is homomorphic to SO(3) $\otimes$ SO(3).

(iv) SO(N) is simple for $N \geq 5$.

Example V *The groups* $\mathrm{U}(N)$, $N \geq 1$

(i) $\mathrm{U}(1)$ is Abelian and therefore not simple.

(ii) For $N \geq 2$, as $\mathrm{u}(N) = \mathrm{u}(1) \oplus \mathrm{su}(N)$ (see Example I of Chapter 9, Section 6) and, as u(l) is Abelian, $\mathrm{U}(N)$ is not semi-simple.

Example VI *The Euclidean group of* $\mathbb{R}^3$
Reference to Example II of Chapter 2, Section 7, shows that the subgroup of pure translations is an Abelian invariant Lie subgroup of this group, which cannot therefore be semi-simple.

3 Complexification

The process of going from a real Lie algebra to a complex Lie algebra is known as "complexification". The most straightforward situation is where the real Lie algebra consists of matrices or linear operators, and the basis elements are linearly independent over the field of *complex* numbers. (This was the situation encountered in Chapter 8, Section 4.) Suppose that $\mathcal{L}$ is an n-dimensional real Lie algebra of matrices with basis $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n$. Theorem I of Chapter 3, Section 1, shows that the only solution of $\sum_{p=1}^{n} \lambda_p \mathbf{a}_p = \mathbf{0}$ with $\lambda_1, \lambda_2, \ldots, \lambda_n$ all *real* is $\lambda_1 = \lambda_2 = \ldots = \lambda_n = 0$. However, it is possible that $\sum_{p=1}^{n} \lambda_p \mathbf{a}_p = \mathbf{0}$ with one or more of $\lambda_1, \lambda_2, \ldots, \lambda_n$ *complex* and non-zero, in which case $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n$ are not linearly independent over the field of *complex numbers* (Example II below provides an demonstration of this behaviour).

Nevertheless, the simplest assumption to make is that $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n$ are linearly independent over the field of *complex* numbers. (For a completely general treatment of complexification, see, for example, Chapter 13, Section 3, of Cornwell (1984).) With this assumption the set of matrices of the form $\sum_{p=1}^{n} \lambda_p \mathbf{a}_p$, where $\lambda_1, \lambda_2, \ldots, \lambda_n$ take arbitrary *complex* values constitute a complex Lie algebra $\widetilde{\mathcal{L}}$, the Lie product of which is given by

$$[\mathbf{a}, \mathbf{b}] = \sum_{p,q,r=1}^{n} \lambda_p \mu_q c_{pq}^r \mathbf{a}_r,$$

where $\mathbf{a} = \sum_{p=1}^{n} \lambda_p \mathbf{a}_p$ and $\mathbf{b} = \sum_{q=1}^{n} \mu_q \mathbf{a}_q$, and where, in $\mathcal{L}$, $[\mathbf{a}_p, \mathbf{a}_q] = \sum_{r=1}^{n} c_{pq}^r \mathbf{a}_r$, c_{pq}^r being the structure constants of $\mathcal{L}$. $\widetilde{\mathcal{L}}$ is then the complexification of $\mathcal{L}$. Clearly $\widetilde{\mathcal{L}}$ (considered as a complex vector space) and $\mathcal{L}$ (considered as a real vector space) have the *same* dimension n. Indeed $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n$ form a basis for both $\mathcal{L}$ and $\widetilde{\mathcal{L}}$, and with this basis both Lie algebras have the same set of structure constants.

Example I *The complexification of* $\mathcal{L} = \mathrm{su}(2)$
As the basis elements $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ of $\mathcal{L} = \mathrm{su}(2)$ defined by Equations (8.30) are linearly independent over the field of complex numbers, by the above

construction the complexification $\widetilde{\mathcal{L}}$ of $\mathcal{L} = \mathrm{su}(2)$ may be taken to be the set of all 2×2 matrices of the form $\sum_{p=1}^{3} \lambda_p \mathbf{a}_p$, where $\lambda_1, \lambda_2, \lambda_3$ are complex. (It should be noted that these are *not* necessarily Hermitian.)

Example II *Problems with the complexification of* $\mathcal{L} = \mathrm{sl}(2, \mathbb{C})$
As noted in Table 10.1. $\mathcal{L} = \mathrm{sl}(2, \mathbb{C})$ is the set of all traceless 2×2 matrices. A convenient basis is

$$\mathbf{a}_1 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \mathbf{a}_2 = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad \mathbf{a}_3 = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix},$$

$$\mathbf{a}_4 = \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}, \quad \mathbf{a}_5 = \begin{bmatrix} 0 & i \\ 0 & 0 \end{bmatrix}, \quad \mathbf{a}_6 = \begin{bmatrix} 0 & 0 \\ i & 0 \end{bmatrix}.$$

These are linearly independent over the real field, but as $\mathbf{a}_4 = i\mathbf{a}_1$, $\mathbf{a}_5 = i\mathbf{a}_2$ and $\mathbf{a}_6 = i\mathbf{a}_3$, they are *not* linearly independent over the field of complex numbers.

Definition *Real form of a complex Lie algebra*
A "real form" of a complex Lie algebra $\mathcal{L}'$ is a real Lie algebra whose complexification $\widetilde{\mathcal{L}}$ is isomorphic to $\mathcal{L}'$.

The following example shows that a complex Lie algebra can have two (or more) real forms that are *not* isomorphic.

Example III $\mathrm{su}(2)$ *and* $\mathrm{sl}(2, \mathbb{R})$ *as real forms of the same complex Lie algebra*
Let $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ and $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ be the bases of $\mathrm{su}(2)$ and $\mathrm{sl}(2, \mathbb{R})$, defined by Equations (8.30) and (11.2) respectively. Then $\mathbf{b}_1 = i\mathbf{a}_1$, $\mathbf{b}_2 = \mathbf{a}_2$ and $\mathbf{b}_3 = i\mathbf{a}_3$, so the complexifications of $\mathrm{su}(2)$ and $\mathrm{sl}(2, \mathbb{R})$ *coincide*. Thus $\mathrm{su}(2)$ and $\mathrm{sl}(2, \mathbb{R})$ are both real forms of the same complex Lie algebra.

This example indicates that the deduction of the real forms of a complex Lie algebra is not a trivial matter, even if the complex Lie algebra is simple. This problem will be examined in Section 10. Nevertheless, some straightforward results do exist in this area, as the following very important theorem shows.

Theorem I Let $\widetilde{\mathcal{L}}$ be the complexification of a real Lie algebra $\mathcal{L}$. Then $\widetilde{\mathcal{L}}$ is semi-simple if and only if $\mathcal{L}$ is semi-simple. Moreover, if $\widetilde{\mathcal{L}}$ is simple then $\mathcal{L}$ is also simple.

Proof See, for example, Chapter 13, Section 3, of Cornwell (1984).

Although $\mathcal{L}$ is necessarily simple if $\widetilde{\mathcal{L}}$ is simple, it should be noted that the converse is *not* true. However, it can be shown that if $\mathcal{L}$ is simple and $\widetilde{\mathcal{L}}$ is not simple, then $\widetilde{\mathcal{L}}$ must be the direct sum of two simple complex Lie algebras that are isomorphic (Gantmacher 1939b).

It can be demonstrated quite easily that every d-dimensional representation of $\mathcal{L}$ provides a d-dimensional representation of its complexification $\widetilde{\mathcal{L}}$, and *vice versa*.

Henceforth every complex semi-simple Lie algebra will be denoted by $\widetilde{\mathcal{L}}$, with $\mathcal{L}$ denoting a real Lie algebra. This notation is justified by the fact that every complex semi-simple Lie algebra is isomorphic to the complexification of some real Lie algebra. (Indeed every such complex Lie algebra is isomorphic to the complexification of at least two non-isomorphic real Lie algebras (see Section 10).)

4 The Cartan subalgebras and roots of semi-simple complex Lie algebras

This section and all the remaining sections of this chapter up to the penultimate section will be devoted to the study of the structure of semi-simple *complex* Lie algebras. The transition back to semi-simple real Lie algebras will be considered in the final section.

The presentation will take the form of a series of theorems, which lead to the construction of the "canonical" form of Weyl (1925, 1926a,b). This facilitates the development (given here in outline only) of the complete classification of all simple complex Lie algebras, which was originally given by Killing (1888, 1889a,b, 1890) and Cartan (1894).

It will become clear in the next chapter on the representation theory of semi-simple Lie algebras that there are very considerable advantages in working with the canonical form, so the construction of this form will be considered in detail for several physically important examples.

Definition *Cartan subalgebra* $\mathcal{H}$
A "Cartan subalgebra" $\mathcal{H}$ of a semi-simple complex Lie algebra $\widetilde{\mathcal{L}}$ is a subalgebra of $\widetilde{\mathcal{L}}$ with the following two properties:

(i) $\mathcal{H}$ is a maximal Abelian subalgebra of $\widetilde{\mathcal{L}}$ (that is, $\mathcal{H}$ is Abelian but every subalgebra of $\widetilde{\mathcal{L}}$ containing $\mathcal{H}$ as a proper subalgebra is not Abelian);

(ii) $\mathbf{ad}(h)$ is completely reducible for every $h \in \mathcal{H}$. (Here $\mathbf{ad}$ denotes the adjoint representation of $\widetilde{\mathcal{L}}$.)

(It is possible to give a definition of a Cartan subalgebra that applies to any Lie algebra, but it is necessarily rather more complicated than that just given above. Nevertheless, it can be shown that the general definition reduces to the above definition in the semi-simple case (see Goto and Grosshans 1978, Helgason 1962, 1978, or Samelson 1969).

It requires a fairly lengthy proof to demonstrate that every semi-simple complex Lie algebra $\widetilde{\mathcal{L}}$ *does* possess at least one Cartan subalgebra (see Helgason 1962, 1978). Also, although it is obvious that any automorphism of

$\widetilde{\mathcal{L}}$ maps a Cartan subalgebra into another Cartan subalgebra, the proof that *any* Cartan subalgebra can be mapped into any other Cartan subalgebra by an automorphism of $\widetilde{\mathcal{L}}$ is more difficult (see Helgason 1962). This latter result implies that all the Cartan subalgebras of a semi-simple Lie algebra have the same dimension, and so permits the following definition.

Definition *The rank of a semi-simple complex Lie algebra*
The "rank" l of a semi-simple complex Lie algebra $\widetilde{\mathcal{L}}$ is defined to be the dimension of its Cartan subalgebras.

Now let $h_1, h_2, \ldots, h_l$ be a basis of a Cartan subalgebra $\mathcal{H}$ of a semi-simple complex Lie algebra $\widetilde{\mathcal{L}}$ of rank l and dimension n. (For the present $h_1, h_2, \ldots, h_l$ may be chosen quite arbitrarily, the only requirement being that they are each members of $\mathcal{H}$ and are linearly independent.) Then, as $\mathcal{H}$ is Abelian, the irreducible representations of $\mathcal{H}$ are all one-dimensional. Consequently the matrices $\mathbf{ad}(h_j)$ for $j = 1, 2, \ldots, l$ must not only be diagonalizable but must be simultaneously diagonalizable. As a similarity transformation applied to **ad** corresponds to a change of basis of $\widetilde{\mathcal{L}}$ (see Chapter 9, Section 5), there exists a basis $h_1, h_2, \ldots, h_l, a'_1, a'_2, \ldots, a'_{n-l}$ of $\widetilde{\mathcal{L}}$ such that

$$[h_j, a'_k] = \alpha_k(h_j) a'_k$$

for $j = 1, 2, \ldots, l$, and $k = 1, 2, \ldots, n - l$, where $\alpha_k(h_j)$ are a set of complex numbers. As $\mathcal{H}$ is Abelian,

$$[h_j, h_k] = 0$$

for $j, k = 1, 2, \ldots, l$. Moreover, as $\mathcal{H}$ is a *maximal* Abelian subalgebra of $\widetilde{\mathcal{L}}$, for each $k = 1, 2, \ldots, n - l$, there must exist at least one $j (= 1, 2, \ldots, l)$ such that $\alpha_k(h_j) \neq 0$.

Now let $h = \sum_{j=1}^{l} \mu_j h_j$ be *any* element of $\mathcal{H}$ and for each $k = 1, 2, \ldots, n-l$, *define* a *linear functional* α_k on $\mathcal{H}$ by

$$\alpha_k(h) = \sum_{j=1}^{l} \mu_j \alpha_k(h_j).$$

(As always (see Appendix B, Section 6), a linear functional on a vector space is completely specified by its values on a basis of that space. Here $\mu_1, \mu_2, \ldots, \mu_l$ are arbitrary complex numbers.) Then for *all* $h \in \mathcal{H}$ and for each $k = 1, 2, \ldots, n - l$, the linear functional α_k is not identically zero (i.e. $\alpha_k(h) \neq 0$ for some $h \in \mathcal{H}$) and

$$[h, a'_k] = \alpha_k(h) a'_k.$$

Each such linear functional is called a "non-zero root" of $\widetilde{\mathcal{L}}$.

It is conceivable that two or more such roots may be identical, that is, possibly $\alpha_k(h) = \alpha_{k'}(h)$ for all $h \in \mathcal{H}$ and $k \neq k'$. In fact the closer examination that follows shows that this *cannot* happen, but the possibility will not be excluded for the present.

For any non-zero root α of $\tilde{\mathcal{L}}$ the set of elements $a_\alpha \in \tilde{\mathcal{L}}$ such that

$$[h, a_\alpha] = \alpha(h) a_\alpha \tag{11.4}$$

(for all $h \in \mathcal{H}$) form a subspace of $\tilde{\mathcal{L}}$ which will be denoted by $\tilde{\mathcal{L}}_\alpha$ and will be called the "root subspace" corresponding to α. Then $\tilde{\mathcal{L}}$ is the vector space direct sum of $\mathcal{H}$ and all the root subspaces $\tilde{\mathcal{L}}_\alpha$ corresponding to non-zero roots.

As $[h, h'] = 0$ for all $h, h' \in \mathcal{H}$, it is sometimes convenient to regard $\mathcal{H}$ as being the subspace of $\tilde{\mathcal{L}}$ corresponding to "zero root" and to write $\mathcal{H} = \tilde{\mathcal{L}}_0$. The set of distinct non-zero roots will be denoted henceforth by Δ.

Theorem I If $a_\alpha \in \tilde{\mathcal{L}}_\alpha$ and $a_\beta \in \tilde{\mathcal{L}}_\beta$, then $[a_\alpha, a_\beta] \in \tilde{\mathcal{L}}_{\alpha+\beta}$ if $\alpha + \beta \in \Delta$, but $[a_\alpha, a_\beta] = 0$ if $\alpha + \beta \notin \Delta$.

Proof By Jacobi's identity (Equation (8.14)), if $h \in \mathcal{H}$, $a_\alpha \in \tilde{\mathcal{L}}_\alpha$ and $a_\beta \in \tilde{\mathcal{L}}_\beta$,

$$[h, [a_\alpha, a_\beta]] + [a_\alpha, [a_\beta, h]] + [a_\beta, [h, a_\alpha]] = 0,$$

so that

$$[h, [a_\alpha, a_\beta]] = \{\alpha(h) + \beta(h)\}[a_\alpha, a_\beta],$$

from which the stated result follows immediately.

The conclusions of the following two theorems are rather technical, but are very useful for deducing the other theorems of the series.

Theorem II If $a_\alpha \in \tilde{\mathcal{L}}_\alpha$ and $a_\beta \in \tilde{\mathcal{L}}_\beta$, and if $\alpha + \beta \neq 0$, then

$$B(a_\alpha, a_\beta) = 0.$$

Proof Suppose that a_γ is any basis element of $\tilde{\mathcal{L}}_\gamma$ for any root γ. Then $(ad(a_\alpha)ad(a_\beta))a_\gamma = [a_\alpha, [a_\beta, a_\gamma]]$, which, by the preceding theorem, is a member of $\tilde{\mathcal{L}}_{\alpha+\beta+\gamma}$ if $\alpha+\beta+\gamma$ is a root, but otherwise is equal to 0. In the first case $\tilde{\mathcal{L}}_{\alpha+\beta+\gamma} \cap \tilde{\mathcal{L}}_\gamma = 0$ if $\alpha+\beta \neq 0$. Thus, in both cases, $(ad(a_\alpha)ad(a_\beta))a_\gamma$ contains no part proportional to a_γ. Hence $\mathrm{tr}\{\mathbf{ad}(a_\alpha)\mathbf{ad}(a_\beta)\} = 0$ if $\alpha + \beta \neq 0$.

In particular, as $\mathcal{H} = \tilde{\mathcal{L}}_0$, it follows that

$$B(h, a_\alpha) = 0 \tag{11.5}$$

for all $h \in \mathcal{H}$ and any $a_\alpha \in \tilde{\mathcal{L}}_\alpha$ ($a \in \Delta$). Also if $a_\alpha \in \tilde{\mathcal{L}}_\alpha$ and $\alpha \neq 0$,

$$B(a_\alpha, a_\alpha) = 0. \tag{11.6}$$

Theorem III The Killing form of $\tilde{\mathcal{L}}$ provides a non-degenerate symmetric bilinear form on $\mathcal{H}$.

Proof All that has to be shown is that the Killing form B of $\widetilde{\mathcal{L}}$ is *non-degenerate on* $\mathcal{H}$, that is, if $h' \in \mathcal{H}$ and $B(h', h) = 0$ for all $h \in \mathcal{H}$ then $h' = 0$, for it is obvious that B is symmetric and bilinear on $\mathcal{H}$. Suppose therefore that $h' \in \mathcal{H}$ and $B(h', h) = 0$ for all $h \in \mathcal{H}$. Then, by Equation (11.5), $B(h', a) = 0$ for all $a \in \widetilde{\mathcal{L}}$, and, as B is non-degenerate on $\widetilde{\mathcal{L}}$ (as $\widetilde{\mathcal{L}}$ is assumed to be semi-simple), it follows that $h' = 0$.

It is now possible to associate with every linear functional $\alpha(h)$ on $\mathcal{H}$, and in particular with each root $\alpha \in \Delta$, a unique element h_α of $\mathcal{H}$ by the definition

$$B(h_\alpha, h) = \alpha(h) \tag{11.7}$$

for all $h \in \mathcal{H}$ (see Theorem I of Appendix B, Section 6). These elements h_α play a very important role in the canonical basis of $\widetilde{\mathcal{L}}$.

If $\alpha(h)$ and $\beta(h)$ are any two linear functionals on $\mathcal{H}$, it follows from Equation (11.7) that

$$h_{\alpha+\beta} = h_\alpha + h_\beta. \tag{11.8}$$

Also, as B is symmetric,

$$\alpha(h_\beta) = \beta(h_\alpha) = B(h_\alpha, h_\beta). \tag{11.9}$$

It is convenient to develop the notation a stage further and define $\langle \alpha, \beta \rangle$ by

$$\langle \alpha, \beta \rangle = B(h_\alpha, h_\beta). \tag{11.10}$$

As B is symmetric,

$$\langle \alpha, \beta \rangle = \langle \beta, \alpha \rangle.$$

(In fact $\langle \alpha, \beta \rangle$ can be regarded as a non-degenerate symmetric bilinear form on the dual space $\mathcal{H}^*$ of $\mathcal{H}$, that is, on the space of all linear functionals of $\mathcal{H}$. Angular brackets are used to emphasize that this is not an inner product.) Then Equation (11.9) can be rewritten as

$$\alpha(h_\beta) = \beta(h_\alpha) = \langle \alpha, \beta \rangle. \tag{11.11}$$

Equation (11.4) then implies that

$$[h_\beta, a_\alpha] = \langle \alpha, \beta \rangle a_\alpha,$$

for all $\beta, \alpha \in \Delta$.

With the basis of $\widetilde{\mathcal{L}}$ chosen so that each basis element is a member of some subspace $\widetilde{\mathcal{L}}_\gamma$, for any $h \in \mathcal{H}$ $\mathbf{ad}(h)$ is a diagonal matrix with zero diagonal elements corresponding to the basis elements of $\widetilde{\mathcal{L}}_0 = \mathcal{H}$ and with diagonal element $\gamma(h)$ corresponding to each basis element $\widetilde{\mathcal{L}}_\gamma$ (for $\gamma \in \Delta$). Thus

$$B(h, h') = \sum_{\gamma \in \Delta} (\dim \widetilde{\mathcal{L}}_\gamma) \gamma(h) \gamma(h') \tag{11.12}$$

for all $h, h' \in \mathcal{H}$. In particular, with $h = h_\alpha$ and $h' = h_\beta$, Equation (11.11) implies that

$$\langle \alpha, \beta \rangle = \sum_{\gamma \in \Delta} (\dim \widetilde{\mathcal{L}}_\gamma) \langle \alpha, \gamma \rangle \langle \beta, \gamma \rangle. \tag{11.13}$$

Theorem IV If $\alpha \in \Delta$ then $-\alpha \in \Delta$.

Proof Suppose $\alpha \in \Delta$, $a_\alpha \in \widetilde{\mathcal{L}}_\alpha$ and $-\alpha \notin \Delta$. Then, by Theorem II above, $B(a_\alpha, a) = 0$ for all $a \in \widetilde{\mathcal{L}}$. As this is not possible because B is non-degenerate, $-\alpha$ must be a non-zero root.

Before proceeding further with the general theory, it is useful to clarify these results by examining some physically important examples.

Example I *The Cartan subalgebra and roots of the complexification* $\widetilde{\mathcal{L}}$ *(=* A_1*) of* $\mathcal{L} = \mathrm{su}(2)$ *(and of* $\mathcal{L} = \mathrm{so}(3)$*)*
As noted earlier, the real Lie algebras su(2) and so(3) are isomorphic (see Example III of Chapter 9, Section 3), so their complexifications are also isomorphic. (They will be denoted by A_1 in the general classification that will be given in Section 7.) For concreteness the argument will be given for $\mathcal{L} = \mathrm{su}(2)$. By Example I of Section 3, the complexification $\widetilde{\mathcal{L}}$ of su(2) can be taken to consist of all 2×2 matrices of the form $\sum_{p=1}^{3} \lambda_p \mathbf{a}_p$, where $\lambda_1, \lambda_2, \lambda_3$ are arbitrary complex numbers and $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ are defined by Equations (8.30).

The subspace of matrices of the form $\lambda_3 \mathbf{a}_3$ may be taken as a Cartan subalgebra $\mathcal{H}$. (This is certainly Abelian, and is *maximal* Abelian because if $\mathbf{a} = \sum_{p=1}^{3} \mu_p \mathbf{a}_p$ is such that $[\mathbf{a}, \lambda_3 \mathbf{a}_3] = \mathbf{0}$ then, by the commutation relations of Equations (8.31), $\mu_1 = \mu_2 = 0$. Moreover, from Example I of Section 2,

$$\mathbf{ad}(\lambda_3 \mathbf{a}_3) = \lambda_3 \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

which is diagonalizable and therefore completely reducible.) Thus the rank l is 1, and $\mathcal{H}$ may be taken to have basis element $\mathbf{h}_1 = \mathbf{a}_3$.

From Equations (8.31),

$$\left.\begin{aligned} [\mathbf{h}_1, (\mathbf{a}_1 + i\mathbf{a}_2)] &= i(\mathbf{a}_1 + i\mathbf{a}_2), \\ [\mathbf{h}_1, (\mathbf{a}_1 - i\mathbf{a}_2)] &= -i(\mathbf{a}_1 - i\mathbf{a}_2), \end{aligned}\right\}$$

so that there are two non-zero roots α_1 and $-\alpha_1$, with $\alpha_1(\mathbf{h}_1) = i$. Thus $\widetilde{\mathcal{L}}_{\alpha_1}$ and $\widetilde{\mathcal{L}}_{-\alpha_1}$ are subspaces of matrices of the form $\lambda(\mathbf{a}_1 + i\mathbf{a}_2)$ and $\mu(\mathbf{a}_1 - i\mathbf{a}_2)$ respectively, λ and μ being arbitrary complex numbers, so that both are one-dimensional.

An explicit expression for $\mathbf{h}_{\alpha_1}$ will now be found. From Equation (11.9), $B(\mathbf{h}_{\alpha_1}, \mathbf{h}_{\alpha_1}) = \alpha_1(\mathbf{h}_{\alpha_1})$, so that with $\mathbf{h}_{\alpha_1} = \kappa \mathbf{h}_1$, $\kappa^2 B(\mathbf{h}_1, \mathbf{h}_1) = \kappa \alpha_1(\mathbf{h}_1)$.

But, from Example I of Section 2, $B(\mathbf{h}_1, \mathbf{h}_1)(= B(\mathbf{a}_3, \mathbf{a}_3)) = -2$, so $\kappa = -\frac{1}{2}i$. Thus

$$\mathbf{h}_{\alpha_1} = \frac{1}{4}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{11.14}$$

It should be noted, as $\langle \alpha_1, \alpha_1 \rangle = \alpha_1(\mathbf{h}_{\alpha_1}) = \kappa\alpha_1(\mathbf{h}_1)$, that

$$\langle \alpha_1, \alpha_1 \rangle = 1/2,$$

which is real, positive and rational.

Example II *The Cartan subalgebra and roots of the complexification* $\widetilde{\mathcal{L}}$ *(=* A_2*) of* $\mathcal{L} = \mathrm{su}(3)$

In his original paper on the SU(3) symmetry scheme for hadrons, Gell-Mann (1962) set up a basis for su(3) and its complexification, which has been widely used in the elementary particle literature ever since. It will be shown in the course of the following analysis how this basis is related to the canonical basis. Gell-Mann (1962) defined eight traceless *Hermitian* matrices $\boldsymbol{\lambda}_1, \boldsymbol{\lambda}_2, \ldots, \boldsymbol{\lambda}_8$ by

$$\boldsymbol{\lambda}_1 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \boldsymbol{\lambda}_2 = \begin{bmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \boldsymbol{\lambda}_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

$$\boldsymbol{\lambda}_4 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad \boldsymbol{\lambda}_5 = \begin{bmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{bmatrix}, \quad \boldsymbol{\lambda}_6 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix},$$

$$\boldsymbol{\lambda}_7 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{bmatrix}, \quad \boldsymbol{\lambda}_8 = (1/\sqrt{3})\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{bmatrix}.$$

These satisfy the commutation relations

$$[\boldsymbol{\lambda}_p, \boldsymbol{\lambda}_q] = \sum_{r=1}^{8} 2if_{pqr}\boldsymbol{\lambda}_r, \tag{11.15}$$

where the f_{pqr} are antisymmetric in all three indices, the non-zero values being listed in Table 11.1.

A convenient basis for the real Lie algebra $\mathcal{L} = \mathrm{su}(3)$ is then provided by the traceless *anti-Hermitian* matrices $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_8$, defined by $\mathbf{a}_p = i\boldsymbol{\lambda}_p$, $p = 1, 2, \ldots, 8$. As these are linearly independent over the field of complex numbers, then $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_8$, or, alternatively, $\boldsymbol{\lambda}_1, \boldsymbol{\lambda}_2, \ldots, \boldsymbol{\lambda}_8$, may be taken as the basis of the complexification $\widetilde{\mathcal{L}}$ $(= A_2)$. Direct calculation using Equation (11.15) shows that

$$B(\mathbf{a}_p, \mathbf{a}_q) = -12\delta_{pq}$$

$(p, q = 1, 2, \ldots, 8)$, the deeper significance of which will be explored in Example II of Section 10. Consequently, if $\mathbf{B}$ is the matrix introduced in Theorem II of Section 2, $\det \mathbf{B} = (-12)^8 \neq 0$, so $\mathcal{L}$ and $\widetilde{\mathcal{L}}$ are semi-simple.

pqr	f_{pqr}
123	1
147	1/2
156	−1/2
246	1/2
257	1/2
345	1/2
367	−1/2
458	$\sqrt{3}/2$
678	$\sqrt{3}/2$

Table 11.1: Non-zero values of the constants f_{pqr} of su(3). The f_{pqr} are antisymmetric under permutations of any two indices.

A convenient choice of Cartan subalgebra is the subspace spanned by $\boldsymbol{\lambda}_3$ and $\boldsymbol{\lambda}_8$, which implies that the rank l is 2. Then, with $\mathbf{h}_1 = \boldsymbol{\lambda}_3$ and $\mathbf{h}_2 = \boldsymbol{\lambda}_8$,

$$\begin{aligned}
&[\mathbf{h}_1, (\boldsymbol{\lambda}_1 + i\boldsymbol{\lambda}_2)] = 2(\boldsymbol{\lambda}_1 + i\boldsymbol{\lambda}_2), && [\mathbf{h}_2, (\boldsymbol{\lambda}_1 + i\boldsymbol{\lambda}_2)] = \mathbf{0},\\
&[\mathbf{h}_1, (\boldsymbol{\lambda}_6 + i\boldsymbol{\lambda}_7)] = -(\boldsymbol{\lambda}_6 + i\boldsymbol{\lambda}_7), && [\mathbf{h}_2, (\boldsymbol{\lambda}_6 + i\boldsymbol{\lambda}_7)] = \sqrt{3}(\boldsymbol{\lambda}_6 + i\boldsymbol{\lambda}_7),\\
&[\mathbf{h}_1, (\boldsymbol{\lambda}_4 + i\boldsymbol{\lambda}_5)] = (\boldsymbol{\lambda}_4 + i\boldsymbol{\lambda}_5), && [\mathbf{h}_2, (\boldsymbol{\lambda}_4 + i\boldsymbol{\lambda}_5)] = \sqrt{3}(\boldsymbol{\lambda}_4 + i\boldsymbol{\lambda}_5),\\
&[\mathbf{h}_1, (\boldsymbol{\lambda}_1 - i\boldsymbol{\lambda}_2)] = -2(\boldsymbol{\lambda}_1 - i\boldsymbol{\lambda}_2), && [\mathbf{h}_2, (\boldsymbol{\lambda}_1 - i\boldsymbol{\lambda}_2)] = \mathbf{0},\\
&[\mathbf{h}_1, (\boldsymbol{\lambda}_6 - i\boldsymbol{\lambda}_7)] = (\boldsymbol{\lambda}_6 - i\boldsymbol{\lambda}_7), && [\mathbf{h}_2, (\boldsymbol{\lambda}_6 - i\boldsymbol{\lambda}_7)] = -\sqrt{3}(\boldsymbol{\lambda}_6 - i\boldsymbol{\lambda}_7),\\
&[\mathbf{h}_1, (\boldsymbol{\lambda}_4 - i\boldsymbol{\lambda}_5)] = -(\boldsymbol{\lambda}_4 - i\boldsymbol{\lambda}_5), && [\mathbf{h}_2, (\boldsymbol{\lambda}_4 - i\boldsymbol{\lambda}_5)] = -\sqrt{3}(\boldsymbol{\lambda}_4 - i\boldsymbol{\lambda}_5).
\end{aligned}$$

Thus there are six non-zero roots: $\alpha_1, \alpha_2, \alpha_3$ and $-\alpha_1, -\alpha_2, -\alpha_3$, with

$$\left.\begin{aligned}
&\alpha_1(\mathbf{h}_1) = 2, && \alpha_1(\mathbf{h}_2) = 0,\\
&\alpha_2(\mathbf{h}_1) = -1, && \alpha_2(\mathbf{h}_2) = \sqrt{3},\\
&\alpha_3(\mathbf{h}_1) = 1, && \alpha_3(\mathbf{h}_2) = \sqrt{3}.
\end{aligned}\right\}$$

Clearly $\widetilde{\mathcal{L}}_{\alpha_1}, \widetilde{\mathcal{L}}_{\alpha_2}, \widetilde{\mathcal{L}}_{\alpha_3}, \widetilde{\mathcal{L}}_{-\alpha_1}, \widetilde{\mathcal{L}}_{-\alpha_2}, \widetilde{\mathcal{L}}_{-\alpha_3}$ are all one-dimensional, with basis elements $(\boldsymbol{\lambda}_1 + i\boldsymbol{\lambda}_2)$, $(\boldsymbol{\lambda}_6 + i\boldsymbol{\lambda}_7)$, $(\boldsymbol{\lambda}_4 + i\boldsymbol{\lambda}_5)$, $(\boldsymbol{\lambda}_1 - i\boldsymbol{\lambda}_2)$, $(\boldsymbol{\lambda}_6 - i\boldsymbol{\lambda}_7)$ and $(\boldsymbol{\lambda}_4 - i\boldsymbol{\lambda}_5)$ respectively. It should be noted that $\alpha_3 = \alpha_1 + \alpha_2$.

It remains to calculate explicit expressions for $\mathbf{h}_{\alpha_1}$, $\mathbf{h}_{\alpha_2}$ and $\mathbf{h}_{\alpha_3}$. Suppose $\mathbf{h}_{\alpha_1} = \kappa_1\mathbf{h}_1 + \kappa_2\mathbf{h}_2$. Then, for $j = 1, 2$, Equation (11.7) with $h = \mathbf{h}_j$ gives $\kappa_1 B(\mathbf{h}_1, \mathbf{h}_j) + \kappa_2 B(\mathbf{h}_2, \mathbf{h}_j) = \alpha_1(\mathbf{h}_j)$, a pair of simultaneous linear equations for κ_1 and κ_2. As $B(\mathbf{a}_p, \mathbf{a}_q) = -12\delta_{pq}$ $(p, q = 1, 2, \ldots, 8)$, it follows that $B(\mathbf{h}_1, \mathbf{h}_1) = B(\mathbf{h}_2, \mathbf{h}_2) = 12$ and $B(\mathbf{h}_1, \mathbf{h}_2) = 0$. Thus $\kappa_1 = \frac{1}{6}$, $\kappa_2 = 0$, and so

$$\mathbf{h}_{\alpha_1} = \frac{1}{6}\mathbf{h}_1 = \frac{1}{6}\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{11.16}$$

Similarly,

$$\mathbf{h}_{\alpha_2} = -\frac{1}{12}\mathbf{h}_1 + \frac{1}{12}\sqrt{3}\mathbf{h}_2 = \frac{1}{6}\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}.$$

Finally, as $\mathbf{h}_{\alpha_3} = \mathbf{h}_{\alpha_1+\alpha_2} = \mathbf{h}_{\alpha_1} + \mathbf{h}_{\alpha_2}$,

$$\mathbf{h}_{\alpha_3} = \frac{1}{12}\mathbf{h}_1 + \frac{1}{12}\sqrt{3}\mathbf{h}_2 = \frac{1}{6}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}.$$

It follows from Definition (11.10) that

$$\left.\begin{array}{ll} \langle\alpha_1,\alpha_1\rangle = \frac{1}{3}, & \langle\alpha_1,\alpha_2\rangle = -\frac{1}{6}, \\ \langle\alpha_2,\alpha_1\rangle = -\frac{1}{6}, & \langle\alpha_2,\alpha_2\rangle = \frac{1}{3}, \end{array}\right\} \tag{11.17}$$

all of which are real and rational, and both $\langle\alpha_1,\alpha_1\rangle$ and $\langle\alpha_2,\alpha_2\rangle$ are also positive. Indeed in this case $\langle\alpha_1,\alpha_1\rangle = \langle\alpha_2,\alpha_2\rangle$. Later developments (in Section 7) will also show the significance of the equality

$$2\langle\alpha_1,\alpha_2\rangle/\langle\alpha_1,\alpha_1\rangle = -1,$$

which is an immediate consequence of Equations (11.17).

5 Properties of roots of semi-simple complex Lie algebras

The series of theorems on roots will now be continued. The notation is the same as in the preceding section.

Theorem I If $a_\alpha \in \widetilde{\mathcal{L}}_\alpha$ and $a_{-\alpha} \in \widetilde{\mathcal{L}}_{-\alpha}$ then

$$[a_\alpha, a_{-\alpha}] = B(a_\alpha, a_{-\alpha})h_\alpha. \tag{11.18}$$

Proof For any $h \in \mathcal{H}$, by part (e) of Theorem I of Section 2,

$$B([a_\alpha, a_{-\alpha}], h) = B(a_\alpha, [a_{-\alpha}, h]).$$

But, by Equations (11.4) and (11.7),

$$[a_{-\alpha}, h] = -[h, a_{-\alpha}] = \alpha(h)a_{-\alpha} = B(h_\alpha, h)a_{-\alpha},$$

so that

$$B([a_\alpha, a_{-\alpha}], h) - B(a_\alpha, a_{-\alpha})B(h_\alpha, h) = 0.$$

That is, for any $h \in \mathcal{H}$,

$$B(\{[a_\alpha, a_{-\alpha}] - B(a_\alpha, a_{-\alpha})h_\alpha\}, h) = 0.$$

As B is non-degenerate, it follows that $\{[a_\alpha, a_{-\alpha}] - B(a_\alpha, a_{-\alpha})h_\alpha\} = 0$.

Theorem II For each $\alpha \in \Delta$ and any $a_\alpha \in \widetilde{\mathcal{L}}_\alpha$, there exists an element $a_{-\alpha}$ of $\widetilde{\mathcal{L}}_{-\alpha}$ such that $B(a_\alpha, a_{-\alpha}) \neq 0$.

Proof Suppose, to the contrary, that for some a_α ($\neq 0$) of $\widetilde{\mathcal{L}}_\alpha$, $B(a_\alpha, a_{-\alpha}) = 0$ for *all* $a_{-\alpha} \in \widetilde{\mathcal{L}}_{-\alpha}$. Then by Theorem II of Section 4, $B(a_\alpha, a) = 0$ for all $a \in \widetilde{\mathcal{L}}$. As the Killing form B is non-degenerate, this implies $a_\alpha = 0$, a contradiction.

This theorem has the very important consequence that (as B is bilinear) for *any* $a_\alpha \in \widetilde{\mathcal{L}}_\alpha$ ($\alpha \in \Delta$) and for *any* complex number B_α, there exists an element $a_{-\alpha} \in \widetilde{\mathcal{L}}_{-\alpha}$ such that $B(a_\alpha, a_{-\alpha}) = B_\alpha$.

Theorem III For every $\alpha, \beta \in \Delta$, the quantities $\langle \alpha, \beta \rangle$ are real and rational. Moreover, for every $\alpha \in \Delta$, $\langle \alpha, \alpha \rangle$ is positive.

Proof See, for example, Appendix E, Section 7, of Cornwell (1984).

Theorem IV $\mathcal{H}$ coincides with the subspace of $\widetilde{\mathcal{L}}$ consisting of all elements of the form $\sum_{\alpha \in \Delta} \mu_\alpha h_\alpha$, where the μ_α take all complex values.

Proof Let $\mathcal{H}'$ be the latter subspace, which is clearly a subspace of $\mathcal{H}$. Suppose that $\mathcal{H}'$ is a *proper* subspace of $\mathcal{H}$. Then there exists a linear functional $\gamma(h)$ of $\mathcal{H}$ such that $\gamma(h)$ is not identically zero on $\mathcal{H}$ but $\gamma(h) = 0$ for all $h \in \mathcal{H}'$. Let h_γ ($\neq 0$) be defined (as in Equation (11.7)) by $B(h_\gamma, h) = \gamma(h)$ for all $h \in \mathcal{H}$. Then, as $\gamma(h_\alpha) = 0$ for all $\alpha \in \Delta$, $B(h_\gamma, h_\alpha) = 0$ for all $\alpha \in \Delta$, and hence, by Equation (11.9), $\alpha(h_\gamma) = 0$ for all $\alpha \in \Delta$. Thus, by Equation (11.4), $[h_\gamma, a] = 0$ for all $a \in \widetilde{\mathcal{L}}$, so h_γ is the basis of a one-dimensional Abelian invariant subalgebra of $\widetilde{\mathcal{L}}$. As $\widetilde{\mathcal{L}}$ is semi-simple, this is impossible, so $\mathcal{H}'$ and $\mathcal{H}$ must coincide.

This theorem implies that from the set of elements h_α ($\alpha \in \Delta$), a subset of l linearly independent elements may be selected and may be taken to form a basis for $\mathcal{H}$. The elements of this set will be denoted by $h_{\beta_1}, h_{\beta_2}, \ldots, h_{\beta_l}$ ($\beta_1, \beta_2, \ldots, \beta_l \in \Delta$). (This set is not unique. For instance, for the complexification $\widetilde{\mathcal{L}}$ ($= A_2$) of su(3), Example II of Section 4 shows that $\beta_1 = \alpha_1$, $\beta_2 = \alpha_2$ gives a basis for $\mathcal{H}$, but one of several alternative bases is given by $\beta_1 = \alpha_1$, $\beta_2 = \alpha_1 + \alpha_2$).

Theorem V *Every* non-zero root α of Δ can be written in the form

$$\alpha = \sum_{j=1}^{l} \kappa_j \beta_j,$$

where the coefficients $\kappa_1, \kappa_2, \ldots, \kappa_l$ are all *real* and rational.

Proof For any $\alpha \in \Delta$, as $h_{\beta_1}, h_{\beta_2}, \ldots, h_{\beta_l}$ form a basis of $\mathcal{H}$, it follows that $h_\alpha = \sum_{j=1}^{l} \kappa_j h_{\beta_j}$, where $\kappa_1, \kappa_2, \ldots, \kappa_l$ are a set of complex numbers. Then

$\alpha = \sum_{j=1}^{l} \kappa_j \beta_j$, so that, for $k = 1, 2, \ldots, l$,

$$\langle \beta_k, \alpha \rangle = \sum_{j=1}^{l} \kappa_j \langle \beta_k, \beta_j \rangle.$$

This is a set of l linear simultaneous algebraic equations for $\kappa_1, \kappa_2, \ldots, \kappa_l$. As the quantities $\langle \beta_k, \alpha \rangle$ and $\langle \beta_k, \beta_j \rangle$ are all real and rational, then so must be $\kappa_1, \kappa_2, \ldots, \kappa_l$.

Let $\mathcal{H}_{\mathbb{R}}$ denote the *real* vector space with basis $h_{\beta_1}, h_{\beta_2}, \ldots, h_{\beta_l}$. The preceding theorem implies that, for any $\alpha \in \Delta$, $h_\alpha = \sum_{j=1}^{l} \kappa_j h_{\beta_j}$, with $\kappa_1, \kappa_2, \ldots, \kappa_l$ real (and rational), so $h_\alpha \in \mathcal{H}_{\mathbb{R}}$ for *all* $\alpha \in \Delta$. Thus $\mathcal{H}_{\mathbb{R}}$ is actually *independent* of the choice of the basis $h_{\beta_1}, h_{\beta_2}, \ldots, h_{\beta_l}$ of $\mathcal{H}$.

Theorem VI For any $\alpha \in \Delta$, $\alpha(h)$ is *real* for all $h \in \mathcal{H}_{\mathbb{R}}$.

Proof Suppose $h \in \mathcal{H}_{\mathbb{R}}$. Then there exists a set of *real* numbers $\mu_1, \mu_2, \ldots, \mu_l$ such that $h = \sum_{j=1}^{l} \mu_j h_{\beta_j}$. Thus

$$\alpha(h) = \sum_{j=1}^{l} \mu_j \alpha(h_{\beta_j}) = \sum_{j=1}^{l} \mu_j \langle \alpha, \beta_j \rangle,$$

which is *real* by Theorem III of this section.

Theorem VII The Killing form B of $\widetilde{\mathcal{L}}$ provides an *inner product* for the *real* vector space $\mathcal{H}_{\mathbb{R}}$.

Proof It has only to be shown that $B(h, h')$ is real for all $h, h' \in \mathcal{H}_{\mathbb{R}}$, and, for all $h \in \mathcal{H}_{\mathbb{R}}$, that $B(h, h)$ is non-negative and that $B(h, h) = 0$ implies that $h = 0$ (see Appendix B, Sections 2 and 5). The first result follows immediately from Equation (11.12) and Theorem VI. Also from Equation (11.12), $B(h, h) = \sum_{\gamma \in \Delta} (\dim \widetilde{\mathcal{L}}_\gamma) \{\gamma(h)\}^2$, which is non-negative as each $\gamma(h)$ is real. Moreover, $B(h, h) = 0$ only if $\gamma(h) = 0$ for *all* $\gamma \in \Delta$, which is only possible if $h = 0$.

Theorem VIII If $\alpha \in \Delta$ then $\dim \widetilde{\mathcal{L}}_\alpha = 1$, and $k\alpha \in \Delta$ only if $k = 1$ or -1.

Proof See, for example, Appendix E, Section 7, of Cornwell (1984).

As a consequence of this theorem, Equation (11.12) simplifies to

$$B(h, h') = \sum_{\gamma \in \Delta} \gamma(h) \gamma(h') \tag{11.19}$$

for all $h, h' \in \mathcal{H}$, and Equation (11.13) reduces to

$$\langle \alpha, \beta \rangle = \sum_{\gamma \in \Delta} \langle \alpha, \gamma \rangle \langle \beta, \gamma \rangle \tag{11.20}$$

for all $\alpha, \beta \in \Delta$.

For each pair of roots α and $-\alpha$ of Δ there exists a *very* useful three-dimensional simple subalgebra of $\widetilde{\mathcal{L}}$ that can be constructed in the following way. *Define* H_α $(\in \mathcal{H})$ by

$$H_\alpha = \{2/\langle\alpha, \alpha\rangle\} h_\alpha, \tag{11.21}$$

and let E_α and $E_{-\alpha}$ be elements of $\widetilde{\mathcal{L}}_\alpha$ and $\widetilde{\mathcal{L}}_{-\alpha}$ respectively such that

$$B(E_\alpha, E_{-\alpha}) = 2/\langle\alpha, \alpha\rangle. \tag{11.22}$$

Then, from Equations (11.4), (11.11), (11.18), (11.21) and (11.22),

$$\left.\begin{array}{lcl} [H_\alpha, E_\alpha] & = & 2E_\alpha, \\ [H_\alpha, E_{-\alpha}] & = & -2E_{-\alpha}, \\ [E_\alpha, E_{-\alpha}] & = & H_\alpha. \end{array}\right\} \tag{11.23}$$

These are precisely the commutation relations of the operators A_3, A_+ and A_- of Equations (10.12), (10.13) and (10.14), which played such an important role in angular momentum theory, the identification being

$$2A_3 \leftrightarrow H_\alpha, \; A_+ \leftrightarrow E_\alpha, \; A_- \leftrightarrow E_{-\alpha}. \tag{11.24}$$

Thus *all* the results on representations obtained in Chapter 10 apply immediately to this subalgebra. This will prove very useful both in proving certain theorems and in constructing explicit representations of $\widetilde{\mathcal{L}}$.

It should be noted that the analogue of Equation (11.8) is not true in general for the elements H_α. That is, in general,

$$H_{\alpha+\beta} \neq H_\alpha + H_\beta,$$

because Equations (11.8) and (11.21) imply that

$$H_{\alpha+\beta} = \{\langle\alpha, \alpha\rangle/\langle\alpha+\beta, \alpha+\beta\rangle\} H_\alpha + \{\langle\beta, \beta\rangle/\langle\alpha+\beta, \alpha+\beta\rangle\} H_\beta.$$

Example I *Application to* $\widetilde{\mathcal{L}} = A_1$, *the complexification of* su(2)
As shown in Example I of Section 4, the complexification $\widetilde{\mathcal{L}} = A_1$ of su(2) has only one pair of non-zero roots, namely α_1 and $-\alpha_1$, and $\langle\alpha_1, \alpha_1\rangle = \frac{1}{2}$. Thus, from Equations (11.14) and (11.21),

$$\mathbf{H}_{\alpha_1} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Let $\mathbf{E}_{\alpha_1} = \kappa(\mathbf{a}_1 + i\mathbf{a}_2)$ and $\mathbf{E}_{-\alpha_1} = \mu(\mathbf{a}_1 - i\mathbf{a}_2)$. Example I of Section 2 then shows that

$$B(\mathbf{E}_{\alpha_1}, \mathbf{E}_{-\alpha_1}) = \kappa\mu B(\mathbf{a}_1 + i\mathbf{a}_2, \mathbf{a}_1 - i\mathbf{a}_2) = -4\kappa\mu,$$

so Equation (11.22) is satisfied with $\kappa\mu = -1$. A convenient choice is $\kappa = \mu = -i$, which gives (by Equations (8.30))

$$\mathbf{E}_{\alpha_1} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad \mathbf{E}_{-\alpha_1} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}.$$

This example shows that, for *every* semi-simple complex Lie algebra $\widetilde{\mathcal{L}}$ and *any* non-zero root α of $\widetilde{\mathcal{L}}$, the elements H_α, E_α and $E_{-\alpha}$ form the basis of a subalgebra that is isomorphic to the complexification A_1 of su(2). Such a subalgebra will henceforth be called an "A_1 subalgebra", but in the mathematical physics literature it is often referred to as an "su(2) subalgebra". (Strictly speaking, this latter terminology is not accurate, as even if Equations (11.23) are taken to be the commutation relations of a real Lie algebra, this real Lie algebra is not isomorphic to su(2) but is another real form of the complexification of su(2). Nevertheless, this slight misuse of language causes no confusion in practice.)

Example II *The A_1 subalgebras (or "su(2) subalgebras") of the complexification $\widetilde{\mathcal{L}}$ (= A_2) of* su(3)

As shown in Example II of Section 4, the complexification $\widetilde{\mathcal{L}}$ (= A_2) of su(3) has three pairs of non-zero roots, namely $(\alpha_1, -\alpha_1)$, $(\alpha_2, -\alpha_2)$ and $(\alpha_3, -\alpha_3)$.

For the first pair, as $\langle \alpha_1, \alpha_1 \rangle = \frac{1}{3}$, Equations (11.16) and (11.21) imply that

$$\mathbf{H}_{\alpha_1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

With $\mathbf{E}_{\alpha_1} = \kappa(\boldsymbol{\lambda}_1 + i\boldsymbol{\lambda}_2)$ and $\mathbf{E}_{-\alpha_1} = \mu(\boldsymbol{\lambda}_1 - i\boldsymbol{\lambda}_2)$, the third commutation relation of Equations (11.23), together with Equation (11.15), gives $\kappa\mu = \frac{1}{4}$. A convenient choice is $\kappa = \mu = \frac{1}{2}$, producing

$$\mathbf{E}_{\alpha_1} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{E}_{-\alpha_1} = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

In the SU(3) symmetry scheme for hadrons this subalgebra is usually called the "I-spin" subalgebra, and a very common notation is defined by

$$I_+ = E_{\alpha_1}, \; I_- = E_{-\alpha_1}, \; I_3 = (1/2)H_{\alpha_1}.$$

Similarly, for the pair $(\alpha_2, -\alpha_2)$,

$$\mathbf{H}_{\alpha_2} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \quad \mathbf{E}_{\alpha_2} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{E}_{-\alpha_2} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}.$$

This subalgebra is called the "U-spin" or "L-spin" subalgebra (De Swart 1963), the identification of generators being

$$U_+ = L_+ = E_{\alpha_2}, \; U_- = L_- = E_{-\alpha_2}, \; U_3 = L_3 = (1/2)H_{\alpha_2}.$$

Finally, for the pair $(\alpha_3, -\alpha_3)$, a similar argument gives

$$\mathbf{H}_{\alpha_3} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \mathbf{E}_{\alpha_3} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \mathbf{E}_{-\alpha_3} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix},$$

the resulting subalgebra being called the "V-spin" or "K-spin" subalgebra (De Swart 1963), the identification of generators in this case being

$$V_+ = K_+ = E_{\alpha_3},\ V_- = K_- = E_{-\alpha_3},\ V_3 = K_3 = -(1/2)H_{\alpha_3}.$$

The next stage in the development involves the concept of a "string" of roots, the usefulness of which will become very clear in Section 7. Several other important results will appear as by-products of this notion.

Definition *The α-string of roots containing β*
Suppose that $\alpha, \beta \in \Delta$. Then the "α-string of roots containing β" is the set of all roots of the form $\beta + k\alpha$, where k is an integer.

Example III *Strings of roots of the complexification $\widetilde{\mathcal{L}}$ $(= A_2)$ of* su(3)
As shown in Example II of Section 4, the non-zero roots of $\widetilde{\mathcal{L}}$ $(= A_2)$ are $\pm\alpha_1$, $\pm\alpha_2$ and $\pm(\alpha_1 + \alpha_2)$. Thus the α_1-string containing α_2 consists of α_2 and $(\alpha_1 + \alpha_2)$, and the α_2-string containing $(\alpha_1 + \alpha_2)$ consists of α_1 and $(\alpha_1 + \alpha_2)$.

Theorem IX Let $\alpha, \beta \in \Delta$. Then there exist two non-negative integers p and q (which depend on α and β) such that $\beta + k\alpha$ is in the α-string containing β for *every* integer k that satisfies the relation $-p \leq k \leq q$. Moreover, p and q are such that

$$p - q = 2\langle\beta, \alpha\rangle / \langle\alpha, \alpha\rangle. \tag{11.25}$$

Also

$$\beta - \{2\langle\beta, \alpha\rangle / \langle\alpha, \alpha\rangle\}\alpha \tag{11.26}$$

is a non-zero root.

Proof See, for example, Appendix E, Section 7, of Cornwell (1984).

Theorem X For all $\alpha, \beta \in \Delta$, $2\langle\beta, \alpha\rangle / \langle\alpha, \alpha\rangle$ can take only the *integral* values $0, \pm 1, \pm 2$ or ± 3. (The quantities $2\langle\beta, \alpha\rangle / \langle\alpha, \alpha\rangle$ are called the "Cartan integers".)

Proof That $2\langle\beta, \alpha\rangle / \langle\alpha, \alpha\rangle$ must be an integer is an immediate consequence of Equation (11.25), as p and q are integers. Clearly, with $\beta = \pm\alpha$, $2\langle\beta, \alpha\rangle / \langle\alpha, \alpha\rangle = \pm 2$. Suppose then that $\beta \neq \pm\alpha$, so that h_α and h_β are linearly independent. As the Killing form B provides an inner product for $\mathcal{H}_{\mathbb{R}}$, applying the Schwarz inequality (see Appendix B, Section 2) gives

$$|B(h_\alpha, h_\beta)|^2 < B(h_\alpha, h_\alpha)\, B(h_\beta, h_\beta).$$

Thus, by Equation (11.10),

$$|\langle\alpha,\beta\rangle|^2 < \langle\alpha,\alpha\rangle\langle\beta,\beta\rangle,$$

so that

$$|2\langle\alpha,\beta\rangle/\langle\alpha,\alpha\rangle|\,|2\langle\alpha,\beta\rangle/\langle\beta,\beta\rangle| < 4,$$

from which it follows that $|2\langle\alpha,\beta\rangle/\langle\alpha,\alpha\rangle|$ can only take values 0, 1, 2 or 3.

The final theorem shows that the Cartan subalgebra and root system together *completely* specify a semi-simple complex Lie algebra (up to isomorphism). As a preliminary, let $\mathcal{H}$ and $\mathcal{H}'$ be two complex vector spaces and suppose that ϕ is a linear mapping of $\mathcal{H}$ onto $\mathcal{H}'$. Then $\alpha'(\phi(h))$ is a linear functional defined on $\mathcal{H}$ if α' is a linear functional defined on $\mathcal{H}'$. (This follows because, for any $h_1, h_2 \in \mathcal{H}$ and any two complex numbers κ_1 and κ_2,

$$\begin{aligned}\alpha'(\phi(\kappa_1 h_1 + \kappa_2 h_2)) &= \alpha'(\kappa_1\phi(h_1) + \kappa_2\phi(h_2)) \text{ (as } \phi \text{ is linear)}\\ &= \kappa_1\alpha'(\phi(h_1)) + \kappa_2\alpha'(\phi(h_2)) \text{ (as } \alpha' \text{ is linear).)}\end{aligned}$$

Theorem XI Suppose that $\widetilde{\mathcal{L}}$ and $\widetilde{\mathcal{L}}'$ are two semi-simple complex Lie algebras with Cartan subalgebras $\mathcal{H}$ and $\mathcal{H}'$ respectively and non-zero root systems Δ and Δ' respectively. If ϕ is a linear mapping of $\mathcal{H}$ onto $\mathcal{H}'$ such that $\alpha'(\phi(h)) \in \Delta$ for every $\alpha' \in \Delta'$, then ϕ can be extended to become an isomorphic mapping of $\widetilde{\mathcal{L}}$ onto $\widetilde{\mathcal{L}}'$.

Proof See, for example, Helgason (1962, 1978) or Varadarajan (1974).

6 The remaining commutation relations

It is now time to examine the commutation relations between elements of $\widetilde{\mathcal{L}}_\alpha$ and $\widetilde{\mathcal{L}}_\beta$, where $\alpha, \beta \in \Delta$ and $\beta \neq -\alpha$. Suppose that α, β, and $\alpha + \beta \in \Delta$, and let e_α, e_β and $e_{\alpha+\beta}$ be basis elements of $\widetilde{\mathcal{L}}_\alpha$, $\widetilde{\mathcal{L}}_\beta$ and $\widetilde{\mathcal{L}}_{\alpha+\beta}$ respectively. Theorem I of Section 4 then implies that there exists a complex number $N_{\alpha,\beta}$ such that

$$[e_\alpha, e_\beta] = N_{\alpha,\beta} e_{\alpha+\beta}. \tag{11.27}$$

Theorem I If α, β and $\alpha + \beta \in \Delta$, then $N_{\alpha,\beta} \neq 0$.

Proof See, for example, Chapter 13, Section 6, of Cornwell (1984).

It will be obvious that the value of $N_{\alpha,\beta}$ depends on the choice of the basis elements e_α, e_β and $e_{\alpha+\beta}$, although it is always true that

$$N_{\beta,\alpha} = -N_{\alpha,\beta}. \tag{11.28}$$

However, Equation (11.6) shows that $B(e_\alpha, e_\alpha) = 0$, so that the Killing form B does *not* provide any natural normalization of e_α. Several different sets of conventions for the choice of the e_α will be found in the mathematics literature, and a detailed discussion of them is given in Chapter 13, Section 6, of Cornwell (1984).

Here attention will be concentrated on just one choice of conventions, *which will be adopted for the rest of this book*, in which for *all* pairs α and $-\alpha$ of Δ,

$$B(e_\alpha, e_{-\alpha}) = -1, \tag{11.29}$$

and for *all* $\alpha, \beta \in \Delta$,

$$N_{-\alpha,-\beta} = N_{\alpha,\beta}. \tag{11.30}$$

With these conventions it can be shown that:

(a) the $N_{\alpha,\beta}$ are all *real*,

(b) if $\alpha, \beta, \gamma \in \Delta$ and $\alpha + \beta + \gamma = 0$, then

$$N_{\alpha,\beta} = N_{\beta,\gamma} = N_{\gamma,\alpha}, \tag{11.31}$$

(c) if $\alpha, \beta, \gamma, \delta \in \Delta$ are such that the sum of no two of them is zero, and if $\alpha + \beta + \gamma + \delta = 0$, then

$$N_{\alpha,\beta}N_{\gamma,\delta} + N_{\beta,\gamma}N_{\alpha,\delta} + N_{\gamma,\alpha}N_{\beta,\delta} = 0, \tag{11.32}$$

(d) for all $\alpha, \beta \in \Delta$,

$$\{N_{\alpha,\beta}\}^2 = \langle\alpha,\alpha\rangle q(p+1)/2, \tag{11.33}$$

where p and q are such that the α-string containing β is $\beta - p\alpha, \ldots, \beta, \ldots, \beta + q\alpha$.

Moreover Equation (11.18) gives

$$[e_\alpha, e_{-\alpha}] = -h_\alpha \tag{11.34}$$

for all $\alpha \in \Delta$. Of course Equation (11.4) is valid with $a_\alpha = e_\alpha$, so that for all $h \in \mathcal{H}$

$$[h, e_\alpha] = \alpha(h)e_\alpha, \tag{11.35}$$

and in particular

$$[h_\beta, e_\alpha] = \alpha(h_\beta)e_\alpha \; (= \langle\alpha,\beta\rangle e_\alpha). \tag{11.36}$$

The basis elements E_α and $E_{-\alpha}$ introduced in Section 5 may be defined in terms of the basis elements e_α and $e_{-\alpha}$ by

$$\left.\begin{aligned} E_\alpha &= \{2/\langle\alpha,\alpha\rangle\}^{1/2}e_\alpha, \\ E_{-\alpha} &= -\{2/\langle\alpha,\alpha\rangle\}^{1/2}e_{-\alpha}. \end{aligned}\right\} \tag{11.37}$$

Then

$$B(E_\alpha, E_{-\alpha}) = 2/\langle\alpha,\alpha\rangle,$$

as in (11.22).

In the case of a Lie algebra of matrices, the argument of Section 10 will show that, after an appropriate similarity transformation if necessary, the elements $\mathbf{h}_\alpha$ of $\mathcal{H}$ may be taken to be diagonal Hermitian matrices, while for each pair α and $-\alpha$ of Δ the matrices $\mathbf{e}_\alpha$ and $\mathbf{e}_{-\alpha}$ may be chosen so that

$$\mathbf{e}_{-\alpha} = -\mathbf{e}_\alpha{}^\dagger, \tag{11.38}$$

and correspondingly, by Equations (11.37),

$$\mathbf{E}_{-\alpha} = \mathbf{E}_\alpha{}^\dagger. \tag{11.39}$$

(Taking the adjoint of $[\mathbf{h}_\beta, \mathbf{e}_\alpha] = \alpha(\mathbf{h}_\beta)\mathbf{e}_\alpha$ gives $[\mathbf{h}_\beta, \mathbf{e}_\alpha{}^\dagger] = -\alpha(\mathbf{h}_\beta)\mathbf{e}_\alpha{}^\dagger$, as $\mathbf{h}_\beta{}^\dagger = \mathbf{h}_\beta$ and $\alpha(\mathbf{h}_\beta)$ $(= \langle\alpha, \beta\rangle)$ is real, implying that $\mathbf{e}_\alpha{}^\dagger$ corresponds to root $-\alpha$. (The argument of Section 10 confirms that, after an appropriate similarity transformation if necessary, $\mathbf{e}_\alpha{}^\dagger$ can be taken to be a member of $\widetilde{\mathcal{L}}$.) Then taking the adjoint of $[\mathbf{e}_\alpha, \mathbf{e}_\beta] = N_{\alpha,\beta}\mathbf{e}_{\alpha+\beta}$ gives $[\mathbf{e}_\alpha{}^\dagger, \mathbf{e}_\beta{}^\dagger] = N_{\alpha,\beta}\mathbf{e}_{\alpha+\beta}{}^\dagger$, so that Equation (11.38) is consistent with the convention of Equation (11.30).) With the choice of convention (11.38), Equation (11.29) becomes $B(\mathbf{e}_\alpha, \mathbf{e}_\alpha{}^\dagger) = 1$, which determines $\mathbf{e}_\alpha$ up to a factor of modulus unity.

Example I *Basis vectors of the complexification* $\widetilde{\mathcal{L}}$ $(= A_2)$ *of* su(3)
As noted in Example II of Section 4, $\widetilde{\mathcal{L}}_{\alpha_1}$, $\widetilde{\mathcal{L}}_{\alpha_2}$, $\widetilde{\mathcal{L}}_{\alpha_1+\alpha_2}$, $\widetilde{\mathcal{L}}_{-\alpha_1}$, $\widetilde{\mathcal{L}}_{-\alpha_2}$ and $\widetilde{\mathcal{L}}_{-(\alpha_1+\alpha_2)}$ have basis elements $(\boldsymbol{\lambda}_1 + i\boldsymbol{\lambda}_2)$, $(\boldsymbol{\lambda}_6 + i\boldsymbol{\lambda}_7)$, $(\boldsymbol{\lambda}_4 + i\boldsymbol{\lambda}_5)$, $(\boldsymbol{\lambda}_1 - i\boldsymbol{\lambda}_2)$, $(\boldsymbol{\lambda}_6 - i\boldsymbol{\lambda}_7)$ and $(\boldsymbol{\lambda}_4 - i\boldsymbol{\lambda}_5)$ respectively. Thus

$$\left.\begin{array}{ll} \mathbf{e}_{\alpha_1} = \kappa_{\alpha_1}(\boldsymbol{\lambda}_1 + i\boldsymbol{\lambda}_2), & \mathbf{e}_{-\alpha_1} = \kappa_{-\alpha_1}(\boldsymbol{\lambda}_1 - i\boldsymbol{\lambda}_2), \\ \mathbf{e}_{\alpha_2} = \kappa_{\alpha_2}(\boldsymbol{\lambda}_6 + i\boldsymbol{\lambda}_7), & \mathbf{e}_{-\alpha_2} = \kappa_{-\alpha_2}(\boldsymbol{\lambda}_6 - i\boldsymbol{\lambda}_7), \\ \mathbf{e}_{(\alpha_1+\alpha_2)} = \kappa_{(\alpha_1+\alpha_2)}(\boldsymbol{\lambda}_4 + i\boldsymbol{\lambda}_5), & \mathbf{e}_{-(\alpha_1+\alpha_2)} = \kappa_{-(\alpha_1+\alpha_2)}(\boldsymbol{\lambda}_4 - i\boldsymbol{\lambda}_5), \end{array}\right\}$$

where $\kappa_{\alpha_1}, \ldots, \kappa_{-(\alpha_1+\alpha_2)}$ are a set of complex numbers. Then, as $B(\boldsymbol{\lambda}_p, \boldsymbol{\lambda}_q) = 12\delta_{pq}$ $(p, q = 1, 2, \ldots, 8)$, the above conventions are satisfied with

$$\kappa_\alpha = \begin{cases} 1/\sqrt{24}, & \text{for } \alpha = \alpha_1, \alpha_2, (\alpha_1 + \alpha_2), \\ -1/\sqrt{24}, & \text{for } \alpha = -\alpha_1, -\alpha_2, -(\alpha_1 + \alpha_2). \end{cases}$$

Consequently

$$\mathbf{e}_{\alpha_1} = (1/\sqrt{6})\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \qquad \mathbf{e}_{-\alpha_1} = -(1/\sqrt{6})\begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

$$\mathbf{e}_{\alpha_2} = (1/\sqrt{6})\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}, \qquad \mathbf{e}_{-\alpha_2} = -(1/\sqrt{6})\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix},$$

$$\mathbf{e}_{(\alpha_1+\alpha_2)} = (1/\sqrt{6})\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{e}_{-(\alpha_1+\alpha_2)} = -(1/\sqrt{6})\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}.$$

With this choice,

$$N_{\alpha_1,\alpha_2} = N_{\alpha_2,-(\alpha_1+\alpha_2)} = N_{-(\alpha_1+\alpha_2),\alpha_1} = 1/\sqrt{6},$$

with the other non-zero structure constants being given by (11.30) and (11.28). The matrices $\mathbf{h}_{\alpha_1}$ and $\mathbf{h}_{\alpha_2}$ of Example II of Section 4 complete the basis.

In the theoretical physics literature (e.g. Behrends *et al.* 1962) a different choice of basis of the Cartan subalgebra $\mathcal{H}$ is often encountered. Theorem VII of Section 5 shows that the Killing form B of $\widetilde{\mathcal{L}}$ provides an inner product for the real vector space $\mathcal{H}_{\mathbb{R}}$. Consequently a basis may be set up in $\mathcal{H}_{\mathbb{R}}$ that is ortho-normal with respect to the Killing form, and this basis is also a basis of $\mathcal{H}$. Thus there exist l elements $H_1, H_2, \ldots, H_l$ of $\mathcal{H}_{\mathbb{R}}$ (and so of $\mathcal{H}$) such that

$$B(H_j, H_k) = \delta_{jk}, \tag{11.40}$$

for $j, k = 1, 2, \ldots, l$. Then, for any linear functional $\alpha(h)$ defined on $\mathcal{H}$ the element h_α ($\in \mathcal{H}$) defined by Equation (11.7) is given by

$$h_\alpha = \sum_{j=1}^{l} \alpha(H_j) H_j. \tag{11.41}$$

(As $H_1, H_2, \ldots, H_l$ form a basis for $\mathcal{H}$, $h_\alpha = \sum_{j=1}^{l} \mu_j^\alpha H_j$ for some set of complex numbers $\mu_1^\alpha, \mu_2^\alpha, \ldots, \mu_l^\alpha$. But, by Equation (11.7), $B(h_\alpha, H_k) = \alpha(H_k)$, so $\sum_{j=1}^{l} \mu_j^\alpha B(H_j, H_k) = \alpha(H_k)$, whence Equation (11.40) implies that $\mu_k^\alpha = \alpha(H_k)$).

The advantage of this basis is that $\langle \alpha, \beta \rangle$ can always be expressed in a particularly simple form. Indeed for any two linear functionals $\alpha(h)$ and $\beta(h)$ defined on $\mathcal{H}$, Equations (11.11) and (11.41) imply that

$$\langle \alpha, \beta \rangle = \sum_{j=1}^{l} \alpha(H_j)\beta(H_j). \tag{11.42}$$

As noted earlier, every linear functional defined on $\mathcal{H}$ is completely specified by its values on a basis of $\mathcal{H}$. In particular, $\alpha(h)$ is completely specified by the set of values $\alpha(H_1), \alpha(H_2), \ldots, \alpha(H_l)$, which, by Theorem VI of Section 5, are all real when α is a root of $\widetilde{\mathcal{L}}$. This set can be written as an l-component vector $\boldsymbol{\alpha}$, that is

$$\boldsymbol{\alpha} = (\alpha(H_1), \alpha(H_2), \ldots, \alpha(H_l)).$$

Consequently, if the scalar product $\boldsymbol{\alpha}.\boldsymbol{\beta}$ of two such l-component vectors $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ is defined by

$$\boldsymbol{\alpha}.\boldsymbol{\beta} = \sum_{j=1}^{l} \alpha(H_j)\beta(H_j),$$

that is, as the inner product of l-dimensional real Euclidean space, Equation (11.42) becomes simply

$$\boldsymbol{\alpha}.\boldsymbol{\beta} = \langle \alpha, \beta \rangle. \tag{11.43}$$

With this choice of basis, Equation (11.35) gives

$$[H_j, e_\alpha] = \alpha(H_j)e_\alpha$$

for each $\alpha \in \Delta$, and Equations (11.34) and (11.41) give

$$[e_\alpha, e_{-\alpha}] = -\sum_{j=1}^{l} \alpha(H_j)H_j$$

for each $\alpha \in \Delta$, both relations involving only components of $\boldsymbol{\alpha}$. These considerations explain why theoretical physicists tend to call $\boldsymbol{\alpha}$ a "root", whereas mathematicians prefer to attach this name to the corresponding linear functional $\alpha(h)$.

It may be noted that as $\mathbf{ad}(H_j)$ is a diagonal matrix with zero diagonal elements corresponding to the basis elements of $\mathcal{H}$ and with diagonal element $\alpha(H_j)$ corresponding to the basis element e_α,

$$B(H_j, H_k) = \sum_{\alpha\in\Delta} \alpha(H_j)\alpha(H_k),$$

so the condition in Equation (11.40) implies that

$$\sum_{\alpha\in\Delta} \alpha(H_j)\alpha(H_k) = \delta_{jk},$$

for $j, k = 1, 2, \ldots, l$.

Example II *Ortho-normal basis of the Cartan subalgebra $\mathcal{H}$ of the complexification $\widetilde{\mathcal{L}}$ (= A_2) of* su(3)
Applying the Schmidt orthogonalization process (see Appendix B, Section 2) to $\phi_j = h_{\alpha_j}$ $(j = 1, 2)$ with $(\phi_j, \phi_k) = B(h_{\alpha_j}, h_{\alpha_k}) = \langle \alpha_j, \alpha_k \rangle$, Equations (11.17) give

$$\left.\begin{array}{rcl} H_1 &=& \sqrt{3}h_{\alpha_1}, \\ H_2 &=& 2(h_{\alpha_2} + \frac{1}{2}h_{\alpha_1}). \end{array}\right\}$$

Thus, using Equations (11.17) again,

$$\left.\begin{array}{rcl} \boldsymbol{\alpha}_1 &=& \frac{1}{6}(2\sqrt{3}, 0), \\ \boldsymbol{\alpha}_2 &=& \frac{1}{6}(-\sqrt{3}, 3), \end{array}\right\}$$

and, using the explicit matrix representations of Example II of Section 4,

$$\left.\begin{array}{rcl} \mathbf{H}_1 &=& (1/2\sqrt{3}) \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix} = (1/2\sqrt{3})\boldsymbol{\lambda}_3, \\ \mathbf{H}_2 &=& (1/6) \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{bmatrix} = (1/2\sqrt{3})\boldsymbol{\lambda}_8. \end{array}\right\}$$

The reader should be warned that there is a complete lack of uniformity of notation in the literature regarding the different choices of bases of $\mathcal{H}$, with the same symbols h_j, h_{α_j}, H_{α_j} and H_j being sometimes defined quite differently by other authors.

7 The simple roots

Let $h_{\beta_1}, h_{\beta_2}, \ldots, h_{\beta_l}$ be a set of l linearly independent elements of $\mathcal{H}$, as defined in Section 5. Then, as shown in Theorem V of Section 5, every non-zero root α of Δ can be written in the form

$$\alpha = \sum_{j=1}^{l} \kappa_j \beta_j, \tag{11.44}$$

with the coefficients $\kappa_1, \kappa_2, \ldots, \kappa_l$ all real and rational.

Definition *Positive root*
A non-zero root α of Δ is said to be "positive" (with respect to the basis $\beta_1, \beta_2, \ldots, \beta_l$) if the first non-vanishing coefficient of the set $\kappa_1, \kappa_2, \ldots, \kappa_l$ appearing in Equation (11.44) is positive.

A similar definition of a "positive linear functional" can obviously be given for *any* linear functional α defined on $\mathcal{H}$ for which Equation (11.44) is valid with the coefficients $\kappa_1, \kappa_2, \ldots, \kappa_l$ all real. For brevity, the statement "α is positive" may be written as "$\alpha > 0$".

Example I *Positive roots of the complexification* $\widetilde{\mathcal{L}}$ *(=* A_2*) of* su(3)
As shown in Example II of Section 4, the non-zero roots of $\widetilde{\mathcal{L}} = A_2$ are $\pm\alpha_1$, $\pm\alpha_2$ and $\pm(\alpha_1 + \alpha_2)$. With respect to $\beta_1 = \alpha_1$, $\beta_2 = \alpha_2$, the positive roots are α_1, α_2 and $\alpha_1 + \alpha_2$. However, with respect to $\beta_1 = \alpha_1$, $\beta_2 = \alpha_1 + \alpha_2$, the positive roots are α_1, $-\alpha_2$ and $\alpha_1 + \alpha_2$, ($-\alpha_2$ being positive as $-\alpha_2 = \alpha_1 - (\alpha_1 + \alpha_2) = \beta_1 - \beta_2$).

This example shows that the question of whether or not a given root $\alpha \in \Delta$ is positive depends entirely on the choice of the basis $\beta_1, \beta_2, \ldots, \beta_l$. Normally once a choice of this basis is made it is adhered to, and with that understanding one can talk of a "positive root" without it being necessary to explicitly make reference to the basis $\beta_1, \beta_2, \ldots, \beta_l$.

Clearly, if $\alpha \in \Delta$ is positive then $-\alpha$ is not positive, so that exactly one half of the set of non-zero roots are positive roots. Also, if $\alpha > 0$ and $\beta > 0$ then $\alpha + \beta > 0$. The set of positive roots (defined relative to some fixed basis $\beta_1, \beta_2, \ldots, \beta_l$) will be denoted by Δ_+.

Definition *Lexicographic ordering of roots*
Let α and β be any two roots of Δ. Then if $(\alpha - \beta) > 0$ one says that $\alpha > \beta$.

Clearly, if $\alpha \neq \beta$ then either $\alpha > \beta$ or $\beta > \alpha$. If $\alpha = \sum_{j=1}^{l} \kappa_j^{\alpha} \beta_j$ and $\beta = \sum_{j=1}^{l} \kappa_j^{\beta} \beta_j$, then $\alpha - \beta = \sum_{j=1}^{l} (\kappa_j^{\alpha} - \kappa_j^{\beta}) \beta_j$. Thus $\alpha > \beta$ if and only if the first non-vanishing coefficient $\kappa_j^{\alpha} - \kappa_j^{\beta}$ is positive. Put another way, $\alpha > \beta$, if, for some s with value $1, 2, \ldots,$ or l, $\kappa_j^{\alpha} = \kappa_j^{\beta}$ for $j = 1, 2, \ldots, s-1$ but $\kappa_s^{\alpha} > \kappa_s^{\beta}$. (The term "lexicographic" is used to describe the ordering

because it corresponds precisely to the conventional ordering of words in a dictionary, where for example "bat" appears before "cat" and "arm" before "art".) Again the lexicographic ordering depends on the choice of the basis $\beta_1, \beta_2, \ldots, \beta_l$.

The lexicographic ordering definition can obviously be extended to any linear functionals defined on $\mathcal{H}$ for which Equation (11.44) is valid with the coefficients $\kappa_1, \kappa_2, \ldots, \kappa_l$ all *real*.

Definition *Simple root of* Δ
A non-zero root α of Δ is said to be "simple" if α is positive but α cannot be expressed in the form $\alpha = \beta + \gamma$, where β and γ are both positive roots of Δ.

Again all these statements are made relative to some chosen basis β_1, β_2, ..., β_l, and whether a given root $\alpha \in \Delta$ is simple depends on this choice, as the following example shows.

Example II *Simple roots of the complexification* $\widetilde{\mathcal{L}}$ *(=* A_2*) of* su(3)
With $\beta_1 = \alpha_1$, $\beta_2 = \alpha_2$, it is obvious that α_1 and α_2 are the only simple roots. However, with $\beta_1 = \alpha_1$, $\beta_2 = \alpha_1 + \alpha_2$, the simple roots are $-\alpha_2$ and $\alpha_1 + \alpha_2$. This follows because with this basis the set of positive roots is α_1, $-\alpha_2$ and $\alpha_1 + \alpha_2$ (see Example I), but $\alpha_1 = (\alpha_1 + \alpha_2) + (-\alpha_2)$, so α_1 cannot be simple, whereas $-\alpha_2$ and $\alpha_1 + \alpha_2$ are simple as they cannot be expressed as the sum of two other positive roots.

For the rest of this section it will be assumed that for each $\widetilde{\mathcal{L}}$ some choice of basis $\beta_1, \beta_2, \ldots, \beta_l$ has been made and is being strictly adhered to. Moreover, the simple roots that correspond to this basis will hereafter be denoted by $\alpha_1, \alpha_2, \ldots, \alpha_l$. (This notation has already been anticipated in the discussions on $\widetilde{\mathcal{L}} = A_1$ and A_2 in the examples above and in the previous three sections. As Example II shows, for $\widetilde{\mathcal{L}} = A_2$ and with the choice $\beta_1 = \alpha_1$, $\beta_2 = \alpha_2$, α_1 and α_2 are indeed simple. Similarly for $\widetilde{\mathcal{L}} = A_1$, with $\beta_1 = \alpha_1$, the root α_1 is positive and simple.)

The first theorem that follows is of a rather technical nature, but the second is of crucial importance, for it shows that the set of simple roots form a basis of $\mathcal{H}^\star$ with very useful properties.

Theorem I If α and β are two simple roots of Δ, and $\alpha \neq \beta$, then

(a) $\alpha - \beta$ is *not* a root of Δ; and

(b) $\langle \alpha, \beta \rangle < 0$.

Proof See, for example, Chapter 13, Section 7, of Cornwell (1984).

Theorem II If $\widetilde{\mathcal{L}}$ has rank l then $\widetilde{\mathcal{L}}$ possesses precisely l simple roots $\alpha_1, \alpha_2, \ldots, \alpha_l$. They form a basis for the dual space $\mathcal{H}^\star$ (the space of all

linear functionals on $\mathcal{H}$). Moreover, if α is any *positive* root of Δ then

$$\alpha = \sum_{j=1}^{l} k_j \alpha_j,$$

where $k_1, k_2, \ldots, k_l$ is a set of *non-negative integers.*

Proof See, for example, Appendix E, Section 9, of Cornwell (1984).

With the properties of the simple roots established, the next stage is to introduce the "Cartan matrix", which plays a crucial role in the developments that follow.

Definition *Cartan matrix* **A**
The "Cartan matrix" **A** of $\widetilde{\mathcal{L}}$ is an $l \times l$ matrix whose elements A_{jk} are defined in terms of the simple roots $\alpha_1, \alpha_2, \ldots, \alpha_l$ of $\widetilde{\mathcal{L}}$ by

$$A_{jk} = \frac{2\langle \alpha_j, \alpha_k \rangle}{\langle \alpha_j, \alpha_j \rangle} \tag{11.45}$$

for $j, k = 1, 2, \ldots, l$.

Clearly $A_{jj} = 2$ for all $j = l, 2, \ldots, l$, while Theorem X of Section 5 and part (b) of Theorem I above together imply that for $j \neq k$ the only possible values of A_{jk} are $0, -1, -2$ or -3. Moreover, $A_{jk} = 0$ if and only if $A_{kj} = 0$. (This follows because $\langle \alpha_j, \alpha_k \rangle = \frac{1}{2} A_{jk} \langle \alpha_j, \alpha_j \rangle$ and $\langle \alpha_k, \alpha_j \rangle (= \langle \alpha_j, \alpha_k \rangle) = \frac{1}{2} A_{kj} \langle \alpha_k, \alpha_k \rangle$. As $\langle \alpha_j, \alpha_j \rangle$ and $\langle \alpha_k, \alpha_k \rangle$ are both non-zero, $A_{jk} = 0$ if and only if $\langle \alpha_j, \alpha_k \rangle = 0$, that is, if and only if $A_{kj} = 0$.) It can be shown that it is always true that $\det \mathbf{A} \neq 0$.

Example III *The Cartan matrices of* $\widetilde{\mathcal{L}} = A_1$ *and* $\widetilde{\mathcal{L}} = A_2$ *(the complexifications of* su(2) *and* su(3))
For $\widetilde{\mathcal{L}} = A_1$, as $l = 1$, **A** is the 1×1 matrix $\mathbf{A} = [2]$. For $\widetilde{\mathcal{L}} = A_2$, Equations (11.17) and (11.45) give

$$\mathbf{A} = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}.$$

As this example shows, it is elementary to construct the Cartan matrix **A** of $\widetilde{\mathcal{L}}$ from a knowledge of the root system of $\widetilde{\mathcal{L}}$. What is very remarkable is that the process can be *reversed.* In fact

(i) it is possible to deduce a *complete* classification of *all* possible Cartan matrices merely from the theorems given above (*without* any *a priori knowledge* of the corresponding Lie algebras); and

(ii) from the Cartan matrix **A** of $\widetilde{\mathcal{L}}$ it is possible to construct the *complete* system of roots Δ of $\widetilde{\mathcal{L}}$, together with the whole set of quantities $\langle \alpha_j, \alpha_k \rangle$ for $j, k = 1, 2, \ldots, l$.

Indeed, as will be shown in Chapter12, the Cartan matrix of $\widetilde{\mathcal{L}}$ also gives the irreducible representations of $\widetilde{\mathcal{L}}$.

This process therefore provides a *complete* classification and specification of *all* the semi-simple complex Lie algebras. As Theorem III of Section 2 shows that every semi-simple complex Lie algebra is the direct sum of simple complex Lie algebras, attention can be concentrated on the Cartan matrices corresponding to the *simple* complex Lie algebras.

No attempt will be made here to give the detailed analysis involved in this classification. (This may be found, for example, in the works of Jacobson (1962), Varadarajan (1974) and Goto and Grosshans (1978).) The argument is facilitated by the introduction for each $\widetilde{\mathcal{L}}$ of its "Dynkin diagram" (Dynkin 1947). In this diagram each simple root is assigned a point (or "vertex") and $A_{jk}A_{kj}$ lines are drawn between the vertices corresponding to α_j and α_k. Moreover, each vertex is assigned a "weight" ω_j, defined by $\omega_j = \omega\langle\alpha_j, \alpha_j\rangle$, where ω is a constant independent of j chosen so that the minimum value in the set $\omega_1, \omega_2, \ldots, \omega_l$ is 1. Then, by Equation (11.45), $\omega_j/\omega_k = A_{kj}/A_{jk}$ (provided $A_{jk} \neq 0$) . As $A_{jk} \leq 0$ for $j \neq k$, it follows that for $j \neq k$

$$A_{jk} = -\{A_{jk}A_{kj}\}^{1/2}\{\omega_k/\omega_j\}^{1/2}, \tag{11.46}$$

so that it is obvious that the Dynkin diagram of $\widetilde{\mathcal{L}}$ determines the Cartan matrix of $\widetilde{\mathcal{L}}$.

The conclusion of the analysis is that there are four infinite sets of complex Lie algebras,

(i) A_l, $l = 1, 2, 3, \ldots$,

(ii) B_l, $l = 1, 2, 3, \ldots$,

(iii) C_l, $l = 1, 2, 3, \ldots$,

(iv) D_l, $l = 3, 4, 5, \ldots$,

that are known as the "classical simple Lie algebras", and there are five others, denoted by E_6, E_7, E_8, F_4 and G_2, which are called the "exceptional simple Lie algebras". In each case the subscript is the rank of the algebra. The Dynkin diagrams are given in Figure 11.1.

The diagrams for A_1, B_1 and C_1 are identical, from which it follows that the Lie algebras A_1, B_1 and C_1 are isomorphic. The diagram for B_2 differs from that for C_2 only in the labelling of the simple roots, so B_2 and C_2 are also isomorphic. The same is also true of A_3 and D_3. Apart from these, all the Dynkin diagrams exhibited correspond to non-isomorphic simple Lie algebras.

(It is permissible to consider the diagram given for D_l when $l = 2$. It reduces to two vertices of weight 1 with no linking lines, from which it follows that D_2 is not simple and is the direct sum of two A_1 algebras.)

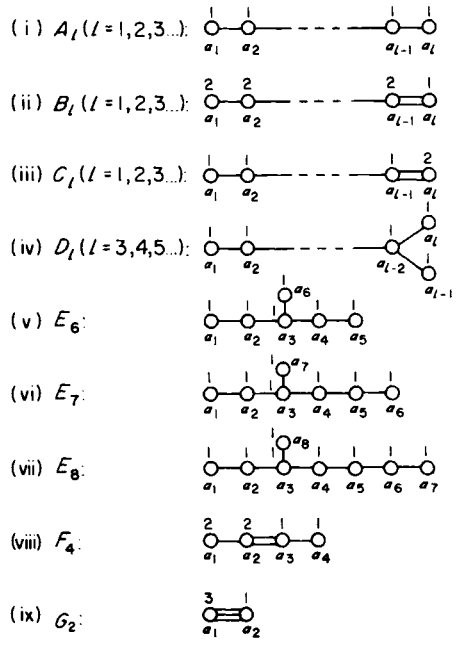

Figure 11.1: Dynkin diagrams of the simple complex Lie algebras. The weight ω_j appears over the vertex labelled by α_j.

Example IV *The Cartan matrices of $\widetilde{\mathcal{L}} = A_1$ and A_2 deduced from their corresponding Dynkin diagrams*

For $\widetilde{\mathcal{L}} = A_1$ the Dynkin diagram is trivial, consisting only of one vertex with weight 1. The only inference is that $l = 1$, which, by Equation (11.45), implies that $\mathbf{A} = [2]$.

For $\widetilde{\mathcal{L}} = A_2$ the Dynkin diagram is given in Figure 11.2. Thus $A_{12}A_{21} = 1$, $\omega_1 = \omega_2 = 1$, so that, by Equation (13.62),

$$\mathbf{A} = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}.$$

It is the equality of the Cartan matrices deduced here with those calculated in Example III that implies that the complexifications $\widetilde{\mathcal{L}}$ of $\mathcal{L} = \mathrm{su}(2)$ and $\mathrm{su}(3)$ are A_1 and A_2 respectively in this scheme of classification. (This has been already anticipated in the notation used in some of the preceding discussions.)

In Appendix D the Cartan matrices are displayed for all the classical simple complex Lie algebras, along with the complete and explicit specifications of all the roots and of the quantities $\langle \alpha_j, \alpha_k \rangle$. (For similar information on the exceptional simple complex Lie algebras, see, for example, Appendix F of

Figure 11.2: Dynkin diagram of A_2.

Cornwell (1984)). The method that enables these quantities to be deduced from the Cartan matrices will not be discussed her, but may be found, for example, in Chapter 13, Section 7, of Cornwell (1984).

8 The Weyl canonical form of $\widetilde{\mathcal{L}}$

It is convenient to now summarize the conclusions of the last four sections by gathering together various commutation relations that have been derived and the assumptions on which they have been based.

Suppose that $\widetilde{\mathcal{L}}$ is a semi-simple complex Lie algebra of rank l. Let $h_{\alpha_1}, h_{\alpha_2}, \ldots, h_{\alpha_l}$ be the elements of the Cartan subalgebra $\mathcal{H}$ corresponding (by Equation (11.7)) to the l *simple* roots $\alpha_1, \alpha_2, \ldots, \alpha_l$ (as defined in Section 7). Let Δ be the set of non-zero roots (as in Section 4), and let e_α be the basis element of the subspace $\widetilde{\mathcal{L}}_\alpha$ chosen so that

$$B(e_\alpha, e_{-\alpha}) = -1 \tag{11.47}$$

(cf. Equation (11.23)). Then

(i) for $j, k = 1, 2, \ldots, l$,

$$[h_{\alpha_j}, h_{\alpha_k}] = 0 \tag{11.48}$$

(as $\mathcal{H}$ is Abelian);

(ii) for any $h \in \mathcal{H}$ and any $\alpha \in \Delta$

$$[h, e_\alpha] = \alpha(h) e_\alpha \tag{11.49}$$

(cf. Equation (11.35)) and in particular, for $h = h_{\alpha_j}$, as $\alpha(h_{\alpha_j}) = \langle \alpha, \alpha_j \rangle$ (by Equation (11.10)),

$$[h_{\alpha_j}, e_\alpha] = \langle \alpha, \alpha_j \rangle e_\alpha \ ; \tag{11.50}$$

(iii) for any $\alpha \in \Delta$,

$$[e_\alpha, e_{-\alpha}] = -h_\alpha \tag{11.51}$$

(cf. Equation (11.34)), so that, with $\alpha = \sum_{j=1}^{l} k_j^\alpha \alpha_j$,

$$[e_\alpha, e_{-\alpha}] = -\sum_{j=1}^{l} k_j^\alpha h_{\alpha_j} \ ; \tag{11.52}$$

(iv) for any $\alpha, \beta \in \Delta$ such that $\beta \neq -\alpha$, if $\alpha + \beta \notin \Delta$,

$$[e_\alpha, e_\beta] = 0, \tag{11.53}$$

while if $\alpha + \beta \in \Delta$,

$$[e_\alpha, e_\beta] = N_{\alpha,\beta} e_{\alpha+\beta}, \tag{11.54}$$

where $N_{\alpha,\beta}$ is a non-zero real number that satisfies

$$N_{-\alpha,-\beta} = N_{\alpha,\beta} \tag{11.55}$$

(cf. Equation (11.30)) and the identities in Equations (11.31) and (11.32), and whose square $\{N_{\alpha,\beta}\}^2$ is given by Equation (11.33).

This canonical form with basis elements h_{α_j} $(j = 1, 2, \ldots, l)$ and e_α $(\alpha \in \Delta)$, and with these commutation relations, is known as the "Weyl canonical form" of $\widetilde{\mathcal{L}}$.

9 The Weyl group of $\widetilde{\mathcal{L}}$

For any linear functional β defined on $\mathcal{H}$ and for any non-zero root $\alpha \in \Delta$, define the linear functional $S_\alpha\beta$ on $\mathcal{H}$ by

$$(S_\alpha\beta)(h) = \beta(h) - \{2\langle\beta, \alpha\rangle / \langle\alpha, \alpha\rangle\}\alpha(h) \tag{11.56}$$

for all $h \in \mathcal{H}$. This defines an *operator* S_α that acts on linear functionals. In particular, if β is a non-zero root of $\widetilde{\mathcal{L}}$, then the last part of Theorem IX of Section 5 shows that $S_\alpha\beta$ is also a non-zero root of $\widetilde{\mathcal{L}}$. Put another way, each S_α maps the set of non-zero roots Δ of $\widetilde{\mathcal{L}}$ into itself. (It will be shown in Chapter 12, Section 2, that a similar result is true of the weights of each representation of $\widetilde{\mathcal{L}}$.)

It is easy to verify that the following properties are valid for any $\alpha \in \Delta$:

(a) in the special case in which $\beta = \alpha$

$$S_\alpha\alpha = -\alpha\,; \tag{11.57}$$

(b) $S_\alpha(S_\alpha\beta) = \beta$ for any linear functional β on $\mathcal{H}$,

(c) for any linear functionals β and γ on $\mathcal{H}$,

$$\langle S_\alpha\beta, S_\alpha\gamma\rangle = \langle\beta, \gamma\rangle\,; \tag{11.58}$$

(d) for any two linear functionals β and γ on $\mathcal{H}$ and any two complex numbers μ and λ,

$$S_\alpha(\lambda\beta + \mu\gamma) = \lambda S_\alpha\beta + \mu S_\alpha\gamma.$$

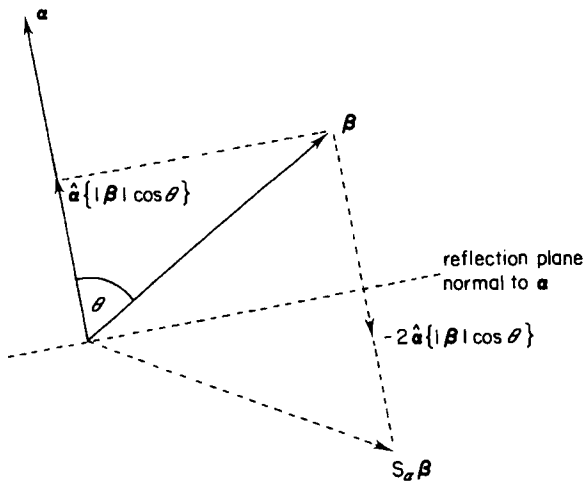

Figure 11.3: The Weyl reflection S_α.

The interpretation of these operators S_α becomes clear if the ortho-normal basis $H_1, H_2, \ldots, H_l$ of $\mathcal{H}$ (introduced in the last part of Section 6) is used. As noted there, each linear functional β on $\mathcal{H}$ has associated with it an l-component vector $\boldsymbol{\beta}$ defined by

$$\boldsymbol{\beta} = (\beta(H_1), \beta(H_2), \ldots, \beta(H_l)).$$

Attention will be concentrated solely on those linear functionals β for which the $\beta(H_j)$ are all real. This includes all the roots (and all the weights) of $\widetilde{\mathcal{L}}$.

Denoting the l-component vector corresponding to $S_\alpha\beta$ by $S_\alpha\boldsymbol{\beta}$, Equations (11.43) and (11.56) give

$$S_\alpha\boldsymbol{\beta} = \boldsymbol{\beta} - \{2(\boldsymbol{\beta}.\boldsymbol{\alpha})/(\boldsymbol{\alpha}.\boldsymbol{\alpha})\}\,\boldsymbol{\alpha}.$$

Let θ be the angle between the vectors $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$, so that $\boldsymbol{\beta}.\boldsymbol{\alpha} = |\boldsymbol{\beta}|\,|\boldsymbol{\alpha}|\cos\theta$, where $|\boldsymbol{\alpha}| = (\boldsymbol{\alpha}.\boldsymbol{\alpha})^{1/2}$ (see Figure 11.3). Then, if $\widehat{\boldsymbol{\alpha}} = \boldsymbol{\alpha}/|\boldsymbol{\alpha}|$ is the unit vector along $\boldsymbol{\alpha}$, $\{2(\boldsymbol{\beta}.\boldsymbol{\alpha})/(\boldsymbol{\alpha}.\boldsymbol{\alpha})\}\boldsymbol{\alpha} = \widehat{\boldsymbol{\alpha}}\{2|\boldsymbol{\beta}|\cos\theta\}$, which is a vector in the direction of $\boldsymbol{\alpha}$ whose magnitude is twice the projection of $\boldsymbol{\beta}$ on $\boldsymbol{\alpha}$. Consequently $S_\alpha\boldsymbol{\beta} = \boldsymbol{\beta} - \widehat{\boldsymbol{\alpha}}\{2|\boldsymbol{\beta}|\cos\theta\}$ is the *reflection* of $\boldsymbol{\beta}$ in the plane perpendicular to $\boldsymbol{\alpha}$ (as is shown clearly in Figure 11.3). As the operators S_α were introduced by Weyl (1925, 1926a,b), they are known as the "Weyl reflections".

With the identity operator E defined by $E\alpha = \alpha$ (for any linear functional α on $\mathcal{H}$) and with products such as $S_\alpha S_\beta$ defined by $S_\alpha S_\beta \gamma = S_\alpha(S_\beta\gamma)$ (for any linear functional γ on $\mathcal{H}$), the set consisting of the identity operator, the Weyl reflections, and all products of Weyl reflections, forms a group, called the "Weyl group", which will be denoted by $\mathcal{W}$. A typical element of $\mathcal{W}$ will be denoted by S. As every element of $\mathcal{W}$ maps the set of non-zero roots of $\widetilde{\mathcal{L}}$ into itself, $\mathcal{W}$ must be a subset of the set of all permutations of the non-zero

roots. Obviously this latter set is finite, so the Weyl group $\mathcal{W}$ of $\widetilde{\mathcal{L}}$ is a *finite* group.

It can be shown (see Jacobson 1962) that every element of $\mathcal{W}$ can be expressed as a product of reflections S_{α_j} associated with the *simple* roots. The construction of $\mathcal{W}$ is helped by the observations that if $S, T \in \mathcal{W}$ then $S = T$ if and only if $S\alpha_j = T\alpha_j$ for every simple root α_j, and that (by Equations (11.45) and 11.56))

$$S_{\alpha_k}\alpha_j = \alpha_j - A_{kj}\alpha_k \tag{11.59}$$

for $j, k = 1, 2, \ldots, l$.

Example I *The Weyl group $\mathcal{W}$ of $\widetilde{\mathcal{L}} = A_2$, the complexification of $\mathcal{L} = \mathrm{su}(3)$* Using the Cartan matrix of Example III of Section 7 and Equation 11.59),

$$\left.\begin{array}{lcl} S_{\alpha_1}\alpha_1 & = & -\alpha_1 \\ S_{\alpha_1}\alpha_2 & = & \alpha_1 + \alpha_2 \end{array}\right\}, \quad \left.\begin{array}{lcl} S_{\alpha_2}\alpha_1 & = & \alpha_1 + \alpha_2 \\ S_{\alpha_2}\alpha_2 & = & -\alpha_2 \end{array}\right\}.$$

It then follows that

$$\left.\begin{array}{lcl} S_{\alpha_2}S_{\alpha_1}\alpha_1 & = & -(\alpha_1 + \alpha_2) \\ S_{\alpha_2}S_{\alpha_1}\alpha_2 & = & \alpha_1 \end{array}\right\}, \quad \left.\begin{array}{lcl} S_{\alpha_1}S_{\alpha_2}\alpha_1 & = & \alpha_2 \\ S_{\alpha_1}S_{\alpha_2}\alpha_2 & = & -(\alpha_1 + \alpha_2) \end{array}\right\},$$

and further that

$$\left.\begin{array}{lcl} S_{\alpha_1}S_{\alpha_2}S_{\alpha_1}\alpha_1 & = & S_{\alpha_2}S_{\alpha_1}S_{\alpha_2}\alpha_1 = -\alpha_2 \\ S_{\alpha_1}S_{\alpha_2}S_{\alpha_1}\alpha_2 & = & S_{\alpha_2}S_{\alpha_1}S_{\alpha_2}\alpha_2 = -\alpha_1 \end{array}\right\}.$$

As every element of $\mathcal{W}$ is a string of products of S_{α_1} and S_{α_2}, and $\{S_{\alpha_1}\}^2 = \{S_{\alpha_2}\}^2 = E$, the fact that $S_{\alpha_1}S_{\alpha_2}S_{\alpha_1} = S_{\alpha_2}S_{\alpha_1}S_{\alpha_2}$ implies that there are no further distinct elements in $\mathcal{W}$. Thus $\mathcal{W}$ is the non-Abelian group of order 6 with elements $\{E, S_{\alpha_1}, S_{\alpha_2}, S_{\alpha_1}S_{\alpha_2}, S_{\alpha_2}S_{\alpha_1}, S_{\alpha_1}S_{\alpha_2}S_{\alpha_1}\}$. (Incidentally, Equation (11.56) shows that $S_{\alpha_1+\alpha_2} = S_{\alpha_1}S_{\alpha_2}S_{\alpha_1}$.)

It is instructive to display these results using the ortho-normal basis H_1, H_2, ..., H_l of $\mathcal{H}$ discussed above. As $l = 2$ here, $\boldsymbol{\beta}$ is a two-component vector which can be taken to be the position vector of a point in a plane, as in Figure 11.4, the reflection planes of the general case becoming reflection lines in this plane. As noted in Example II of Section 6, $\boldsymbol{\alpha}_1 = (1/\sqrt{3})(1, 0)$, $\boldsymbol{\alpha}_2 = (1/2\sqrt{3})(-1, \sqrt{3})$, and so $\boldsymbol{\alpha}_1 + \boldsymbol{\alpha}_2 = (1/2\sqrt{3})(1, \sqrt{3})$, so the reflection lines normal to $\boldsymbol{\alpha}_1$, $\boldsymbol{\alpha}_2$ and $\boldsymbol{\alpha}_1 + \boldsymbol{\alpha}_2$ have directions $(0, 1)$, $\frac{1}{2}(\sqrt{3}, 1)$ and $\frac{1}{2}(\sqrt{3}, -1)$ respectively. If $\boldsymbol{\beta}$ does not lie on a reflection line, the six distinct elements S of $\mathcal{W}$ acting on $\boldsymbol{\beta}$ produce six distinct vectors $S\boldsymbol{\beta}$. However, if $\boldsymbol{\beta}$ lies on a reflection line and $\boldsymbol{\beta} \neq \mathbf{0}$, the set $\{S\boldsymbol{\beta} \mid S \in \mathcal{W}\}$ contains only three members, while if $\boldsymbol{\beta} = \mathbf{0}$ then $\{S\boldsymbol{\beta} \mid S \in \mathcal{W}\}$ contains only the one member $\mathbf{0}$.

The following two theorems give two other useful properties of Weyl reflections.

Theorem I If α is a positive root and $\alpha \neq \alpha_j$, then $S_{\alpha_j}\alpha > 0$.

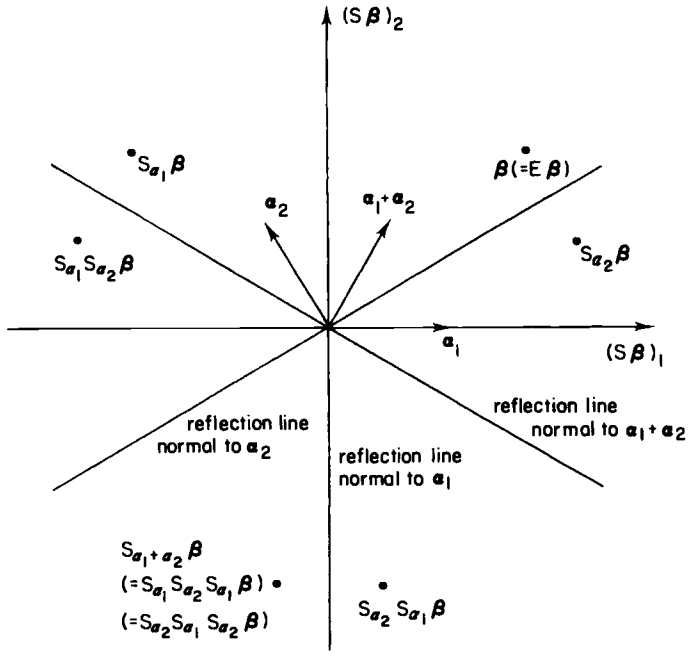

Figure 11.4: The actions of the elements S of the Weyl group $\mathcal{W}$ for $\widetilde{\mathcal{L}} = A_2$ on a general 2-component vector corresponding to a linear functional β on $\mathcal{H}$.

Proof Suppose that $\alpha = \sum_{i=1}^{l} k_i \alpha_i$. Then it follows that

$$\begin{aligned} S_{\alpha_j}\alpha &= \alpha - \{2\langle\alpha,\alpha_j\rangle/\langle\alpha_j,\alpha_j\rangle\}\alpha_j \\ &= \sum_{i=1,i\neq j}^{l} k_i\alpha_i + \{k_j - 2\langle\alpha,\alpha_j\rangle/\langle\alpha_j,\alpha_j\rangle\}\alpha_j. \end{aligned}$$

If $\alpha \neq \alpha_j$ and α is a positive root then, as $\kappa\alpha_j$ is not a root (except when $\kappa = 1, -1$ or 0), at least one of the coefficients k_i must be positive for $i \neq j$. Theorem II of Section 7 then implies that $S_{\alpha_j}\alpha$ must be positive.

Theorem II If $S_{\alpha_j}\alpha = S_{\alpha_j}\beta$ for some $j = 1, 2, \ldots, l$, then $\alpha = \beta$.

Proof If $S_{\alpha_j}\alpha = S_{\alpha_j}\beta$, Equation (11.56) implies that

$$\alpha - \beta = \{2\langle\alpha-\beta,\alpha_j\rangle/\langle\alpha_j,\alpha_j\rangle\}\alpha_j.$$

Thus $\alpha = \beta + \kappa\alpha_j$, where κ is some complex number. Substituting back gives $\kappa\alpha_j = \{2\langle\kappa\alpha_j,\alpha_j\rangle/\langle\alpha_j,\alpha_j\rangle\}\alpha_j = 2\kappa\alpha_j$, so $\kappa = 0$, implying that $\alpha = \beta$.

These two theorems lead to a result that will prove useful in Chapter 12, Section 3:

Theorem III If $\delta = \frac{1}{2}\sum_{\alpha\in\Delta_+}\alpha$, then

$$\langle\delta,\alpha_j\rangle = \frac{1}{2}\langle\alpha_j,\alpha_j\rangle \tag{11.60}$$

for all $j = 1,2,\ldots,l$.

Proof For any $j = 1,2,\ldots,l$, Theorems I and II imply that S_{α_j} maps the set of positive roots (excluding α_j) into the set of positive roots (excluding α_j), so

$$\begin{aligned} S_{\alpha_j}\delta &= \frac{1}{2}\sum_{\alpha\in\Delta_+,\ \alpha\neq\alpha_j} S_{\alpha_j}\alpha + \frac{1}{2}S_{\alpha_j}\alpha_j \\ &= \frac{1}{2}\sum_{\alpha\in\Delta_+,\ \alpha\neq\alpha_j} \alpha - \frac{1}{2}\alpha_j \text{ (by Equation (11.57))} \\ &= \delta - \alpha_j. \end{aligned}$$

Then, by Equation (11.58), $\langle S_{\alpha_j}\delta, S_{\alpha_j}\alpha_j\rangle = \langle\delta,\alpha_j\rangle$, so that $\langle\delta-\alpha_j,-\alpha_j\rangle = \langle\delta,\alpha_j\rangle$, and hence $2\langle\delta,-\alpha_j\rangle = \langle\alpha_j,\alpha_j\rangle$.

The order of $\mathcal{W}$ for each classical simple complex Lie algebra is listed in Appendix D. (The corresponding orders for the exceptional simple complex Lie algebras may be found, for example, in Appendix F of Cornwell (1984).)

10 Semi-simple real Lie algebras

The process of complexification, that is, of passing from a real Lie algebra $\mathcal{L}$ to its associated complex Lie algebra $\tilde{\mathcal{L}}$, was described in Section 3. The opposite procedure will now be considered for the case in which $\tilde{\mathcal{L}}$ is semi-simple. In outline the procedure is quite straightforward, for if $\tilde{\mathcal{L}}$ is a complex Lie algebra, with the basis elements $a_1, a_2, \ldots, a_n$ of $\tilde{\mathcal{L}}$ chosen so that the structure constants c_{pq}^r are all *real*, then *real* linear combinations of $a_1, a_2, \ldots$ and a_n form a real Lie algebra that is one of the "real forms" of $\tilde{\mathcal{L}}$. The problems essentially lie in constructing all the bases of $\tilde{\mathcal{L}}$ with the required property.

There are essentially two stages in this construction. The first is to set up the "compact" real form of the complex Lie algebra $\tilde{\mathcal{L}}$, and the second is to deduce the "non-compact" real forms from the compact real form. The construction and properties of the compact real form will be considered here in some detail, for these properties have wide implications. In particular, a remarkable result of Weyl shows that the compactness or otherwise of a semi-simple Lie *group* can be tested by *algebraic* properties of its associated real Lie *algebra*. Amongst other consequences, this result permits many of

the properties of unitary representations of compact semi-simple Lie groups to be carried over to non-unitary representations of non-compact semi-simple Lie groups, the discussion in Chapter 12, Section 1, of complete reducibility being a good example.

The treatment of non-compact real forms here will be confined to an explicit listing of all the simple non-compact real forms corresponding to classical semi-simple complex Lie algebras, but the method of construction, which is largely due to Cartan (1914, 1929) and Gantmacher (1939a,b), will be omitted. (A full account (using the involutive automorphisms of the compact real forms) appears, for example, in Chapter 14 of Cornwell (1984)).

Definition *Compact and non-compact semi-simple real Lie algebras*
A semi-simple real Lie algebra $\mathcal{L}$ is said to be "compact" if its Killing form is *negative definite* (that is, if $B(a,a) < 0$ for all $a \in \mathcal{L}$ such that $a \neq 0$), and is said to be "non-compact" otherwise.

This terminology is used because compact semi-simple real Lie algebras correspond to compact Lie groups, as will be shown in Theorem III below. (The words "compact" and "non-compact" do *not* describe the topology of $\mathcal{L}$ *itself*, which, being a vector space of dimension n, is homomorphic to the whole of $\mathbb{R}^n$, which is unbounded and consequently always non-compact in the usual topology on $\mathbb{R}^n$.)

Example I $\mathcal{L} = \mathrm{su}(2)$ *as a compact semi-simple real Lie algebra*
Example I of Section 2, shows that for $\mathcal{L} = \mathrm{su}(2)$, $B(\mathbf{a}_p, \mathbf{a}_q) = -2\delta_{pq}$ for $p, q = 1, 2, 3$. Thus, for a general element $\mathbf{a}$ of su(2), writing $\mathbf{a} = \sum_{p=1}^{3} \mu_p \mathbf{a}_p$ with μ_1, μ_2, μ_3 all real, it follows that $B(\mathbf{a}, \mathbf{a}) = -2\sum_{p=1}^{3} \mu_p^2$, so that $B(\mathbf{a}, \mathbf{a}) < 0$ for all $\mathbf{a} \neq \mathbf{0}$. Thus su(2) is a *compact* Lie algebra.

As noted previously, su(2) is the real Lie algebra of the Lie group SU(2), which is a *compact* Lie *group* (see Example III of Chapter 3, Section 3). This provides a particular example of the general theorem stated below as Theorem III.

If $\mathcal{L}$ is a compact semi-simple real Lie algebra, then with (a, b) *defined* for all $a, b \in \mathcal{L}$ by

$$(a, b) = -B(a, b), \tag{11.61}$$

it follows that (a, b) is an *inner product* and $\mathcal{L}$ is an inner product space (see Appendix B, Section 2). As usual, it is then possible to set up ortho-normal sets of basis elements in $\mathcal{L}$. Then, if $a_1, a_2, \ldots, a_n$ is such an ortho-normal set,

$$(a_p, a_q) = -B(a_p, a_q) = \delta_{pq}, \tag{11.62}$$

for $p, q = 1, 2, \ldots, n$.

The following two technical results will become useful in the subsequent development.

Theorem I If $a_1, a_2, \ldots, a_n$ is an ortho-normal basis of a compact semi-simple real Lie algebra $\mathcal{L}$, then the *adjoint* representation of $\mathcal{L}$ defined relative to this basis consists of *antisymmetric* matrices. Put another way, with this basis the structure constants c^r_{pq} are *antisymmetric* with respect to interchanges of *all* pairs of indices (p,q), (q,r) and (r,p), i.e.

$$c^r_{pq} = -c^r_{qp} = -c^q_{pr} = c^q_{rp} = -c^p_{rq} = c^p_{qr}. \tag{11.63}$$

Proof By part (e) of Theorem I of Section 2, for any $a \in \mathcal{L}$ and $p,q = 1,2,\ldots,n$, $B([a_p,a],a_q) = B(a_p,[a,a_q])$. Thus, by Equations (9.14) and the linearity of B,

$$-\sum_{r=1}^{n}\{\mathbf{ad}(a)\}_{rp}B(a_r,a_q) = \sum_{r=1}^{n}\{\mathbf{ad}(a)\}_{rq}B(a_p,a_r),$$

from which it follows by Equation (11.62 that $\{\mathbf{ad}(a)\}_{qp} = -\{\mathbf{ad}(a)\}_{pq}$.

The relation $c^r_{pq} = -c^r_{qp}$ applies for any basis of any Lie algebra, while the other relations in Equations (11.63) are a consequence of the fact that $\{\mathbf{ad}(a_p)\}_{rq} = c^r_{pq}$ (Equation (9.37)).

Theorem II If $\mathcal{L}'$ is a semi-simple real subalgebra of a semisimple real Lie algebra $\mathcal{L}$, then $\mathcal{L}'$ is compact if $\mathcal{L}$ is compact.

Proof See, for example, Appendix E, Section 10, of Cornwell (1984).

The remarkable theorem of Weyl may now be stated:

Theorem III A connected semi-simple linear *Lie group* $\mathcal{G}$ is *compact* if and only if its corresponding *real Lie algebra* $\mathcal{L}$ is *compact* (that is, if and only if the Killing form of $\mathcal{L}$ is *negative definite*).

Proof See, for example, Appendix E, Section 10, of Cornwell (1984).

The most significant point is that this theorem provides a purely *Lie algebraic* criterion for the corresponding Lie *groups* to be compact. It should be noted that this is *only* valid in the *semi-simple* case. Indeed, it has already been noted in Example II of Chapter 9, Section 3, that the Abelian *non-compact* Lie group $\mathbb{R}_+$ and the Abelian *compact* Lie group SO(2) have *isomorphic* real Lie algebras. Consequently for Abelian groups there can be no Lie algebraic criterion for compactness.

The following theorem shows that *every* semi-simple complex Lie algebra $\widetilde{\mathcal{L}}$ has a *compact* real form $\mathcal{L}$ derivable from $\widetilde{\mathcal{L}}$ in a very straightforward manner.

Theorem IV For each semi-simple complex Lie algebra $\widetilde{\mathcal{L}}$, if h_{α_j} $(j = 1,2,\ldots,l)$ and $e_\alpha, e_{-\alpha}$ $(\alpha \in \Delta_+)$ are the basis elements of the Weyl canonical

form, then the set of elements

$$\left.\begin{array}{c} ih_{\alpha_j} \text{ (for } j = 1, 2, \ldots, l), \\ e_\alpha + e_{-\alpha} \text{ (for each } \alpha \in \Delta_+), \\ i(e_\alpha - e_{-\alpha}) \text{ (for each } \alpha \in \Delta_+) \end{array}\right\}$$

form the basis of a *compact* semi-simple real Lie algebra, which will be denoted by $\mathcal{L}_c$, and which will be called a "compact real form" of $\widetilde{\mathcal{L}}$.

Proof See, for example, Appendix E, Section 10, of Cornwell (1984).

Clearly $\mathcal{L}_c$ consists of all elements of the form

$$a = i\sum_{j=1}^{l} \mu_j h_{\alpha_j} + \sum_{\alpha \in \Delta_+} \{x_\alpha(e_\alpha + e_{-\alpha}) + iy_\alpha(e_\alpha - e_{-\alpha})\},$$

where the μ_j, x_α and y_α are all real. Writing $z_\alpha = x_\alpha + iy_\alpha$, so that z_α is a complex number, a typical element $a \in \mathcal{L}_c$ can be expressed as

$$a = i\sum_{j=1}^{l} \mu_j h_{\alpha_j} + \sum_{\alpha \in \Delta_+} \{z_\alpha e_\alpha + z_\alpha^* e_{-\alpha}\}. \tag{11.64}$$

It can be shown that any two compact real forms of $\widetilde{\mathcal{L}}$ are isomorphic, so $\mathcal{L}_c$ is unique up to isomorphism, and may be referred to as "*the* compact real form" of $\widetilde{\mathcal{L}}$.

It is easily verified that the following elements provide a natural *ortho-normal* basis for $\mathcal{L}_c$ with respect to the inner product of Equation (11.61):

$$\left.\begin{array}{c} iH_j \text{ (for } j = 1, 2, \ldots, l), \\ (1/\sqrt{2})(e_\alpha + e_{-\alpha}) \text{ (for each } \alpha \in \Delta_+), \\ (1/\sqrt{2})i(e_\alpha - e_{-\alpha}) \text{ (for each } \alpha \in \Delta_+), \end{array}\right\}$$

$H_1, H_2, \ldots, H_l$ being the ortho-normal basis of $\mathcal{H}$ (i.e. $B(H_j, H_k) = \delta_{jk}$ for $j, k = 1, 2, \ldots, l$ (see Section 6)) and e_α the basis element of $\widetilde{\mathcal{L}}_\alpha$ in the Weyl canonical basis.

In the case of Lie algebras of matrices, as every representation of a compact Lie group is equivalent to a *unitary* representation, the matrices of the corresponding compact real Lie algebra $\mathcal{L}_c$ can (by part (f) of Theorem IV of Chapter 9, Section 4) be taken to be *anti-Hermitian*. The previous theorem then implies that

$$\mathbf{h}_\alpha{}^\dagger = \mathbf{h}_\alpha$$

and

$$\mathbf{e}_\alpha{}^\dagger = -\mathbf{e}_{-\alpha}$$

for all $\alpha \in \Delta$ (as mentioned earlier in Section 6).

Example II *Ortho-normal basis for the compact real form* $\mathcal{L}_c = \mathrm{su}(3)$ *of* $\widetilde{\mathcal{L}} = A_2$

The canonical basis of the complex Lie algebra $\widetilde{\mathcal{L}} = A_2$ has been constructed in Example II of Section 4, in terms of the Gell-Mann matrices $\boldsymbol{\lambda}_1, \boldsymbol{\lambda}_2, \ldots, \boldsymbol{\lambda}_8$. Using this basis and the results of Examples I and II of Section 6, it follows that the *ortho-normal* basis of the compact real form $\mathcal{L}_c$ of $\widetilde{\mathcal{L}} = A_2$ constructed by the above prescription is

$$\begin{aligned}
i\mathbf{H}_1 &= (i\sqrt{3}/6)\boldsymbol{\lambda}_3, \\
i\mathbf{H}_2 &= (i\sqrt{3}/6)\boldsymbol{\lambda}_8, \\
(1/\sqrt{2})(\mathbf{e}_{\alpha_1} + \mathbf{e}_{-\alpha_1}) &= (i\sqrt{3}/6)\boldsymbol{\lambda}_2, \\
(1/\sqrt{2})i(\mathbf{e}_{\alpha_1} - \mathbf{e}_{-\alpha_1}) &= (i\sqrt{3}/6)\boldsymbol{\lambda}_1, \\
(1/\sqrt{2})(\mathbf{e}_{\alpha_2} + \mathbf{e}_{-\alpha_2}) &= (i\sqrt{3}/6)\boldsymbol{\lambda}_7, \\
(1/\sqrt{2})i(\mathbf{e}_{\alpha_2} - \mathbf{e}_{-\alpha_2}) &= (i\sqrt{3}/6)\boldsymbol{\lambda}_6, \\
(1/\sqrt{2})(\mathbf{e}_{\alpha_1+\alpha_2} + \mathbf{e}_{-(\alpha_1+\alpha_2)}) &= (i\sqrt{3}/6)\boldsymbol{\lambda}_5, \\
(1/\sqrt{2})i(\mathbf{e}_{\alpha_1+\alpha_2} - \mathbf{e}_{-(\alpha_1+\alpha_2)}) &= (i\sqrt{3}/6)\boldsymbol{\lambda}_4.
\end{aligned}$$

As the basis of $\mathcal{L} = \mathrm{su}(3)$ chosen in Example II of Section 4 was $\mathbf{a}_p = i\boldsymbol{\lambda}_p$, $p = 1, 2, \ldots, 8$, it follows that the compact real form $\mathcal{L}_c$ of $\widetilde{\mathcal{L}} = A_2$ constructed according to Theorem IV above is *precisely* the real Lie algebra $\mathcal{L} = \mathrm{su}(3)$, and the *ortho-normal* basis of $\mathcal{L}_c$ is provided by $(\sqrt{3}/6)\mathbf{a}_p$, $p = 1, 2, \ldots, 8$ (i.e. the ortho-normal basis differs from the original basis merely by a *common* factor $\sqrt{3}/6$). Consequently

$$B(\mathbf{a}_p, \mathbf{a}_q) = -(6/\sqrt{3})^2 \delta_{pq} = -12\delta_{pq}$$

for $p, q = 1, 2, \ldots, 8$, precisely as noted in Example II of Section 4. Moreover, Theorem I above shows that with this basis the structure constants c^r_{pq} are *antisymmetric* in all pairs of indices, which is certainly so, as (with $\mathbf{a}_p = i\boldsymbol{\lambda}_p$) $c^r_{pq} = -2f_{pqr}$, f_{pqr} being defined in Equation (11.15).

For the classical simple complex Lie algebras A_l, B_l, C_l and D_l the corresponding *compact* real forms are (see Table 8.1):

(a) for $\widetilde{\mathcal{L}} = A_l$, $\mathcal{L}_c = \mathrm{su}(l+1)$, $l = 1, 2, \ldots$

(b) for $\widetilde{\mathcal{L}} = B_l$, $\mathcal{L}_c = \mathrm{so}(2l+1)$, $l = 1, 2, \ldots$

(c) for $\widetilde{\mathcal{L}} = C_l$, $\mathcal{L}_c = \mathrm{sp}(l)$, $l = 1, 2, \ldots$

(d) for $\widetilde{\mathcal{L}} = D_l$, $\mathcal{L}_c = \mathrm{so}(2l)$, $l = 3, 4, \ldots$

(The last-mentioned result applies also to $\widetilde{\mathcal{L}} = D_2$ (which is semisimple but not simple), the corresponding compact real form being $\mathcal{L}_c = \mathrm{so}(4)$ (which is also semi-simple but not simple). See, for example, Appendix G, Section 2(b), of Cornwell (1984) for details.)

The isomorphic mappings between A_1, B_1 and C_1 (noted in Section 7) imply that their compact real forms su(2), so(3) and sp(1) are isomorphic.

Similarly, so(5) and sp(2) are isomorphic as a result of the isomorphism between B_2 and C_2, and su(4) and so(6) are isomorphic because A_3 and D_3 are isomorphic. This in turn implies homomorphic mappings between the corresponding linear Lie groups. For example, there exist homomorphic mappings of SU(2) onto SO(3) and of SU(4) onto SO(6).

For the classical simple complex Lie algebras A_l, B_l, C_l and D_l the corresponding *non-compact* real forms are (see Table 8.1):

(a) $\widetilde{\mathcal{L}} = A_l$ (for $l = 1, 2, \ldots$) has non-compact real forms:

  (i) $\mathcal{L} = \mathrm{su}(l+1-p, p)$ for $p = 1, \ldots, [\frac{1}{2}(l+1)]$,

  (ii) $\mathcal{L} = \mathrm{sl}(l+1, \mathbb{R})$,

  (iii) $\mathcal{L} = \mathrm{su}^*(l+1)$ for l odd only;

(b) $\widetilde{\mathcal{L}} = B_l$ (for $l = 1, 2, \ldots$) has non-compact real forms:
$\mathrm{so}(2l+1-2p, 2p)$ for $p = 1, \ldots, l$;

(c) $\widetilde{\mathcal{L}} = C_l$ (for $l = 1, 2, \ldots$) has non-compact real forms:

  (i) $\mathcal{L} = \mathrm{sp}(p, l-p)$ for $p = 1, \ldots, [\frac{1}{2}l]$,

  (ii) $\mathcal{L} = \mathrm{sp}(l, \mathbb{R})$;

(d) $\widetilde{\mathcal{L}} = D_l$ (for $l = 1, 2, \ldots$) has non-compact real forms:

  (i) $\mathcal{L} = \mathrm{so}(2l-2p, 2p)$ for $p = 1, \ldots, [\frac{1}{2}l]$,

  (ii) $\mathcal{L} = \mathrm{so}(2l-2p+1, 2p+1)$ for $p = 1, \ldots, [\frac{1}{2}l]$,

  (iii) $\mathcal{L} = \mathrm{so}^*(2l)$.

Here $[a]$ denotes the largest integer not greater than a.

Realizations in terms of matrices with complex entries have been given for all the compact and non-compact real forms of the exceptional simple complex Lie algebras E_6, E_7, E_8, F_4 and G_2 by Cartan (1914) and Gantmacher (1939b).

In addition to the above simple real Lie algebras that are generated from *simple* complex Lie algebras, there also exist the non-compact simple real Lie algebras that are generated from *non-simple* complex Lie algebras of the form $\widetilde{\mathcal{L}}_1 \oplus \widetilde{\mathcal{L}}_2$, where $\widetilde{\mathcal{L}}_1$ and $\widetilde{\mathcal{L}}_2$ are *isomorphic* simple complex Lie algebras. The resulting real forms for the classical algebras are:

(a) for $\widetilde{\mathcal{L}} = A_l \oplus A_l$, $\mathcal{L} = \mathrm{sl}(l+1, \mathbb{C})$, $l = 1, 2, \ldots$

(b) for $\widetilde{\mathcal{L}} = B_l \oplus B_l$, $\mathcal{L} = \mathrm{so}(2l+1, \mathbb{C})$, $l = 1, 2, \ldots$

(c) for $\widetilde{\mathcal{L}} = C_l \oplus C_l$, $\mathcal{L} = \mathrm{sp}(l, \mathbb{C})$, $l = 1, 2, \ldots$

(d) for $\widetilde{\mathcal{L}} = D_l \oplus D_l$, $\mathcal{L} = \mathrm{so}(2l, \mathbb{C})$, $l = 3, 4, \ldots$

Again, Table 8.1 contains the specifications of these Lie algebras.

The following sets of non-compact real forms are isomorphic:

(i) $su(1,1) \approx sl(2,\mathbb{R}) \approx so(1,2) \approx sp(1,\mathbb{R})$,

(ii) $so(3,2) \approx sp(2,\mathbb{R})$,

(iii) $so(1,4) \approx sp(1,1)$,

(iv) $su(2,2) \approx so(4,2)$,

(v) $su(3,1) \approx so^*(6)$,

(vi) $so(6,2) \approx so^*(8)$,

(vii) $sl(4,\mathbb{R}) \approx so(3,3)$,

(viii) $su^*(4) \approx so(5,1)$,

(ix) $su(l+1-p,p) \approx su(p,l+1-p)$ for $p = 1,\ldots,[\frac{1}{2}(l+1)]$,

(x) $so(2l+1-2p,2p) \approx so(2p,2l+1-2p)$ for $p = 1,\ldots,l$;

(xi) $so(2l-2p,2p) \approx so(2p,2l-2p)$ for $p = 1,\ldots,[\frac{1}{2}l]$,

(xii) $so(2l-2p+1,2p+1) \approx so(2p+1,2l-2p+1)$ for $p = 1,\ldots,[\frac{1}{2}l]$,

(xiii) $sp(p,l-p) \approx sp(l-p,p)$ for $p = 1,\ldots,[\frac{1}{2}l]$,

(xiv) $sl(2,\mathbb{C}) \approx so(3,\mathbb{C}) \approx sp(1,\mathbb{C}) \approx so(3,1)$,

(xv) $so(5,\mathbb{C}) \approx sp(2,\mathbb{C})$,

(xvi) $sl(4,\mathbb{C}) \approx so(6,\mathbb{C})$.

(The origins of these isomorphisms are discussed, for example, in Chapter 14 of Cornwell (1984).)

Chapter 12

Representations of Semi-simple Lie Algebras

1 Some basic ideas

The key idea in the representation theory of semi-simple complex Lie algebras is that of the "weights". These are introduced in Section 2, where it will be shown that they have very similar properties to the "roots" of Chapter 11, and are related to them in several ways. Section 3 demonstrates how *every* irreducible representation can be determined from its "highest weight", and how the highest weights themselves are to be found. A detailed study is made in Section 4 of the irreducible representations of A_2 (the complexification of su(3)), which not only demonstrate all the general features, but are of great importance in physical applications. Finally, in Section 5 the related idea of Casimir operators will be introduced.

For a description of methods available for the explicit determination of all the matrices of a representation, the calculation of Clebsch-Gordan series and coefficients, and the specification of irreducible representations by Young tableaux, see, for example, Chapter 16 of Cornwell (1984). The computer programme "SimpLie^{TM}" developed by Moody *et al* (1996) is very useful for carrying out such calculations.

The close connection between the representations of a semi-simple complex Lie algebra, the representations of its various real forms, and the representations of the Lie groups associated with these real Lie algebras means that certain statements proved in one situation can be readily transferred to the others. The following two theorems are interesting not merely for the results that are stated, but also because they can be proved using this line of argument.

Theorem I Every reducible representation of a semi-simple real or complex Lie algebra is *completely* reducible.

Proof See, for example, Chapter 15, Section 1, of Cornwell (1984).

Theorem II Every reducible representation of a connected semi-simple Lie group is *completely* reducible.

Proof This follows immediately from the previous theorem and part (d) of Theorem IV of Chapter 9, Section 4.

2 The weights of a representation

Consider a representation $\mathbf{\Gamma}$ of dimension d of a semi-simple complex Lie algebra $\widetilde{\mathcal{L}}$. Because $\mathbf{\Gamma}$ provides a representation of the compact form $\mathcal{L}_c$ of $\widetilde{\mathcal{L}}$ (see Chapter 11, Section 10), on $\mathcal{L}_c$ the representation $\mathbf{\Gamma}$ is equivalent to a representation by anti-Hermitian matrices. Thus, for any $h \in \mathcal{H}_{\mathbb{R}}$, as $ih \in \mathcal{L}_c$, $\mathbf{\Gamma}(ih)$ is diagonalizable and consequently $\mathbf{\Gamma}(h)$ is diagonalizable for all $h \in \mathcal{H}_{\mathbb{R}}$. Moreover, the matrices $\mathbf{\Gamma}(h)$ for each $h \in \mathcal{H}$ may be diagonalized by the *same* similarity transformation. Henceforth it will be assumed that any necessary similarity transformation has already been applied, so that $\mathbf{\Gamma}(h)$ is a *diagonal* matrix for each $h \in \mathcal{H}$.

Consider the diagonal elements $\Gamma(h)_{jj}$ for some fixed j ($j = 1, 2, \ldots, d$). As $\mathbf{\Gamma}(ah + bh') = a\mathbf{\Gamma}(h) + b\mathbf{\Gamma}(h')$ for all $h, h' \in \mathcal{H}$ and any complex numbers a and b, it follows that

$$\Gamma(ah + bh')_{jj} = a\Gamma(h)_{jj} + b\Gamma(h')_{jj}.$$

Thus the diagonal elements $\Gamma(h)_{jj}$ are *linear functionals* defined on $\mathcal{H}$. These linear functionals are called the "weights" of the representation, so that a d-dimensional representation possesses d weights, some of which may be identical.

In terms of modules (see Chapter 9, Section 4), suppose that ψ_1, ψ_2, ..., ψ_d form a basis of the carrier space V of the representation $\mathbf{\Gamma}$ and that $\Phi(a)$ is the operator defined for each $a \in \widetilde{\mathcal{L}}$ by

$$\Phi(a)\psi_j = \sum_{k=1}^{d} \Gamma(a)_{kj}\psi_k$$

for $j = 1, 2, \ldots, d$. Then, for each $h \in \mathcal{H}$, as $\mathbf{\Gamma}(h)$ is diagonal,

$$\Phi(h)\psi_j = \Gamma(h)_{jj}\psi_j \tag{12.1}$$

for $j = 1, 2, \ldots, d$. Thus for each $j = 1, 2, \ldots, d$, and for all $h \in \mathcal{H}$, $\Gamma(h)_{jj}$ is an *eigenvalue* of the operator $\Phi(h)$, the corresponding *eigenvector* being ψ_j.

Let $\lambda_j(h) = \Gamma(h)_{jj}$ define the weight λ_j corresponding to the jth position in the representation. Denoting the corresponding eigenvector ψ_j by $\psi(\lambda_j)$, Equation (12.1) becomes

$$\Phi(h)\psi(\lambda_j) = \lambda_j(h)\psi(\lambda_j), \tag{12.2}$$

for $j = 1, 2, \ldots, d$. When this position is unimportant the index j may be omitted, so that an arbitrary weight of the representation will be denoted by λ. If the weight λ appears $m(\lambda)$ times in the representation, $m(\lambda)$ is said to be the "multiplicity" of λ. If $m(\lambda) = 1$ then λ is described as a "*simple* weight" of the representation. Later examples will show that weights need not be simple, even for irreducible representations. With this simplification of notation, Equation (12.2) can be written as

$$\Phi(h)\psi(\lambda) = \lambda(h)\psi(\lambda) \tag{12.3}$$

for all $h \in \mathcal{H}$, $\psi(\lambda)$ being any eigenvector of $\Phi(h)$ with eigenvalue $\lambda(h)$. The multiplicity $m(\lambda)$ is then the dimension of the subspace of V spanned by the eigenvectors $\psi(\lambda)$.

Example I *The adjoint representation of* $\widetilde{\mathcal{L}}$
Let the basis elements $a_1, a_2, \ldots, a_n$ of $\widetilde{\mathcal{L}}$ be chosen to be $h_{\alpha_1}, h_{\alpha_2}, \ldots, h_{\alpha_l}$, together with e_α, for each $\alpha \in \Delta$. Then, by Equation (9.36) with $a = h$, it follows that $\mathbf{ad}(h)$ is diagonal for each $h \in \mathcal{H}$, the diagonal element corresponding to h_{α_j} being 0 and the diagonal element corresponding to e_α being $\alpha(h)$. Thus each non-zero root α of $\widetilde{\mathcal{L}}$ is a weight of the adjoint representation of $\widetilde{\mathcal{L}}$ and, as $\dim \widetilde{\mathcal{L}}_\alpha = 1$, each such weight is simple. The only other weight λ of the adjoint representation is such that $\lambda(h) = 0$ for all $h \in \mathcal{H}$, and this has multiplicity l.

Example II *Weights of a three-dimensional representation of the complexification* $\widetilde{\mathcal{L}}(= A_2)$ *of* su(3)
Consider the explicit three-dimensional representation of $\widetilde{\mathcal{L}} = A_2$ constructed in Example II of Chapter 11, Section 4. By inspection,

$$\left.\begin{array}{ll} \lambda_1(h_{\alpha_1}) = \frac{1}{6}, & \lambda_1(h_{\alpha_2}) = 0, \\ \lambda_2(h_{\alpha_1}) = -\frac{1}{6}, & \lambda_2(h_{\alpha_2}) = \frac{1}{6}, \\ \lambda_3(h_{\alpha_1}) = 0, & \lambda_3(h_{\alpha_2}) = -\frac{1}{6}, \end{array}\right\}$$

so the three weights λ_1, λ_2 and λ_3 are all simple. It is interesting to note for future reference that, as $\alpha_j(h_{\alpha_k}) = \langle \alpha_j, \alpha_k \rangle$, Equations (11.17) imply that for $h = h_{\alpha_1}$ and h_{α_2},

$$\left.\begin{array}{l} \lambda_1(h) = \frac{2}{3}\alpha_1(h) + \frac{1}{3}\alpha_2(h), \\ \lambda_2(h) = \lambda_1(h) - \alpha_1(h), \\ \lambda_3(h) = \lambda_1(h) - \alpha_1(h) - \alpha_2(h), \end{array}\right\} \tag{12.4}$$

from which it follows that Equations (12.4) are true for *all* $h \in \mathcal{H}$.

It is now possible to derive some simple but important results.

Theorem I If λ is a weight of a representation, then $\lambda + \alpha$ is also a weight of the same representation for each $\alpha \in \Delta$ such that $\Phi(e_\alpha)\psi(\lambda) \neq 0$.

Proof As $[h, e_\alpha] = \alpha(h)e_\alpha$, then $[\Phi(h), \Phi(e_\alpha)] = \alpha(h)\Phi(e_\alpha)$. Consequently, as

$$\Phi(h)\{\Phi(e_\alpha)\psi(\lambda)\} = [\Phi(h), \Phi(e_\alpha)]\psi(\lambda) + \Phi(e_\alpha)\{\Phi(h)\psi(\lambda)\},$$

Equation (12.3) implies that

$$\Phi(h)\{\Phi(e_\alpha)\psi(\lambda)\} = (\alpha(h) + \lambda(h))\{\Phi(e_\alpha)\psi(\lambda)\},$$

so $\Phi(e_\alpha)\psi(\lambda)$ is an eigenvector of $\Phi(h)$ with eigenvalue $\alpha(h) + \lambda(h)$, provided that $\Phi(e_\alpha)\psi(\lambda) \neq 0$.

Theorem II For any weight λ of any representation of $\widetilde{\mathcal{L}}$ and for any root α of Δ, $2\langle\lambda, \alpha\rangle/\langle\alpha, \alpha\rangle$ is an *integer.*

Proof Let $\mathbf{\Gamma}$ be any representation of $\widetilde{\mathcal{L}}$ and let λ be any weight of $\mathbf{\Gamma}$. Consider the three-dimensional A_1 subalgebra with basis H_α, E_α and $E_{-\alpha}$ defined in Equations (11.21) and (11.22), whose commutation relations are given by Equations (11.23). As noted in Chapter 10, Section 3, every irreducible representation of this subalgebra is equivalent to a representation in which the matrix representing H_α is diagonal and has only *integral* diagonal entries. But $\mathbf{\Gamma}$ provides a representation of this subalgebra, which must be equivalent to a direct sum of such irreducible representations. Thus the diagonal elements of $\mathbf{\Gamma}(H_\alpha)$ must all be integers, so $\lambda(H_\alpha)$ is an integer. However, by Equation (11.21), $\lambda(H_\alpha) = \{2/\langle\alpha, \alpha\rangle\}\lambda(h_\alpha) = 2\langle\lambda, \alpha\rangle/\langle\alpha, \alpha\rangle$, from which the quoted result follows.

Theorem III Every weight λ can be written in terms of the simple roots $\alpha_1, \alpha_2, \ldots, \alpha_l$:

$$\lambda = \sum_{j=1}^{l} \mu_j \alpha_j, \tag{12.5}$$

where the coefficients μ_j are all *real* and rational. Consequently $\lambda(h)$ is *real* for each $h \in \mathcal{H}_{\mathbb{R}}$.

Proof Theorem II of Chapter 11, Section 7, shows that $\alpha_1, \alpha_2, \ldots, \alpha_l$ form a basis for $\mathcal{H}^*$, so any linear functional λ can certainly be written in the form of Equation (12.5) for some set of complex numbers $\mu_1, \mu_2, \ldots, \mu_l$. All that has to be shown is that these are real and rational if λ is a weight. However, for each $\alpha \in \Delta$, by Equation (11.21),

$$2\langle\lambda, \alpha\rangle/\langle\alpha, \alpha\rangle = \lambda(H_\alpha) = \sum_{j=1}^{l} \mu_j \alpha_j(H_\alpha) = \sum_{j=1}^{l} \mu_j \{2\langle\alpha_j, \alpha\rangle/\langle\alpha, \alpha\rangle\}.$$

The previous theorem shows that the left-hand side is an integer, while Theorem X of Chapter 11, Section 5, demonstrates that $2\langle\alpha_j, \alpha\rangle/\langle\alpha, \alpha\rangle$ is also an integer for each $j = 1, 2, \ldots, l$. As this is so for *every* $\alpha \in \Delta$, $\mu_1, \mu_2, \ldots, \mu_l$ must be real and rational. Finally, for $h \in \mathcal{H}_{\mathbb{R}}$, $\lambda(h) = \sum_{j=1}^{l} \mu_j \alpha_j(h)$, which

is real, as $\alpha_j(h)$ is real for all $j = 1, 2, \ldots, l$, by Theorem VI of Chapter 11, Section 5.

Theorem IV For each root $\alpha \in \Delta$ and each weight λ of a representation $\mathbf{\Gamma}$ of $\widetilde{\mathcal{L}}$, *define* the linear functional $S_\alpha\lambda$ on $\mathcal{H}$ by

$$(S_\alpha\lambda)(h) = \lambda(h) - \{2\langle\lambda, \alpha\rangle/\langle\alpha, \alpha\rangle\}\alpha(h) \tag{12.6}$$

for all $h \in \mathcal{H}$. Then $S_\alpha\lambda$ is also a weight of the representation $\mathbf{\Gamma}$ with the *same* multiplicity as λ, i.e.

$$m(S_\alpha\lambda) = m(\lambda).$$

Proof See, for example, Chapter 14, Section 2, of Cornwell (1984).

The weight $S_\alpha\lambda$ will be recognized as being a *Weyl reflection* of the weight λ (see Chapter 11, Section 9), so the above theorem states that any Weyl reflection of any weight is a weight with the same multiplicity. Repeated application gives the result that $S\lambda$ is also a weight with same multiplicity as λ for *every* element S of the Weyl group $\mathcal{W}$.

In displaying the symmetries of weights in connection with the Weyl group, it is particularly convenient to use the ortho-normal basis $H_1, H_2, \ldots, H_l$ of $\mathcal{H}$ introduced at the end of Chapter 11, Section 6, and discussed further in Chapter 11, Section 9. Then to every weight λ there corresponds an l-component vector $\boldsymbol{\lambda}$ given by

$$\boldsymbol{\lambda} = (\lambda(H_1), \lambda(H_2), \ldots, \lambda(H_l)),$$

the l-component vector corresponding to $S\lambda$ being denoted by $S\boldsymbol{\lambda}$. Of course, by Equation (12.3),

$$\Phi(H_j)\psi(\lambda) = \lambda(H_j)\psi(\lambda) \tag{12.7}$$

for $j = 1, 2, \ldots, l$, so the components of $\boldsymbol{\lambda}$ are the simultaneous eigenvalues of $\Phi(H_1), \Phi(H_2), \ldots, \Phi(H_l)$.

The concept of a "string" can be extended from roots to weights and produces a generalization of Theorem IX of Chapter 11, Section 5.

Definition *The α-string of weights containing λ*
Suppose that α is a root of $\widetilde{\mathcal{L}}$ and λ is a weight of some representation of $\widetilde{\mathcal{L}}$. Then the "α-string of weights containing λ" is the set of all weights of that representation of the form $\lambda + k\alpha$, where k is an integer.

Theorem V Let α be a non-zero root of $\widetilde{\mathcal{L}}$ and λ a weight of some representation of $\widetilde{\mathcal{L}}$. Then there exist two non-negative integers p and q (which depend on α and λ) such that $\lambda + k\alpha$ is in the α-string containing λ for *every* integer k that satisfies the relations $-p \leq k \leq q$. Moreover, p and q are such that

$$p - q = 2\langle\lambda, \alpha\rangle/\langle\alpha, \alpha\rangle. \tag{12.8}$$

Proof See, for example, Chapter 15, Section 2, of Cornwell (1984).

It should be noted that the weights in the α-string containing λ need *not* have the same multiplicity.

As noted in Chapter 11, Section 10, if the basis $a_1, a_2, \ldots, a_l$ of $\tilde{\mathcal{L}}$ is taken to be ih_{α_j} $(j = 1, 2, \ldots, l)$ together with $(e_\alpha + e_{-\alpha})$ and $i(e_\alpha - e_{-\alpha})$ (for all $\alpha \in \Delta_+$), the structure constants are all *real*, and this basis is also the basis of the compact real form $\mathcal{L}_c$ of $\tilde{\mathcal{L}}$. Thus, if $\mathbf{\Gamma}$ is a d-dimensional representation of $\tilde{\mathcal{L}}$, *define* the matrices $\mathbf{\Gamma}^\star(a_j)$ for each of *these* basis elements a_j by $\mathbf{\Gamma}^\star(a_j) = \{\mathbf{\Gamma}(a_j)\}^\star$ $(j = 1, 2, \ldots, n)$. Extending this to the whole of $\tilde{\mathcal{L}}$ by defining $\mathbf{\Gamma}^\star(\sum_{j=1}^n \mu_j a_j)$ to be $\sum_{j=1}^n \mu_j \mathbf{\Gamma}^\star(a_j)$ for any set of complex numbers $\mu_1, \mu_2, \ldots, \mu_l$, it is obvious that these matrices $\mathbf{\Gamma}^\star$ form a representation of $\tilde{\mathcal{L}}$ of dimension d, and $\mathbf{\Gamma}^\star$ is irreducible if and only if $\mathbf{\Gamma}$ is irreducible. The notation here reflects the fact that the matrices $\mathbf{\Gamma}^\star$ provide a representation of the compact real Lie algebra $\mathcal{L}_c$ that is the complex conjugate of that provided by $\mathbf{\Gamma}$. However, it should be noted that $\{\mathbf{\Gamma}(\sum_{j=1}^n \mu_j a_j)\}^\star = \sum_{j=1}^n \mu_j^\star \mathbf{\Gamma}(a_j)^\star = \sum_{j=1}^n \mu_j^\star \mathbf{\Gamma}^\star(a_j)$, which is not equal to $\mathbf{\Gamma}^\star(\sum_{j=1}^n \mu_j a_j)$ *unless* $\mu_1, \mu_2, \ldots, \mu_l$ are all *real*. Consequently the description of $\mathbf{\Gamma}^\star$ as being the "complex conjugate" of the representation $\mathbf{\Gamma}$ has to be applied with caution, but is nevertheless very useful and widely adopted.

Theorem VI λ is a weight of the representation $\mathbf{\Gamma}$ of $\tilde{\mathcal{L}}$ if and only if $-\lambda$ is a weight of $\mathbf{\Gamma}^\star$. Moreover, the multiplicity of λ in $\mathbf{\Gamma}$ is the same as that of $-\lambda$ in $\mathbf{\Gamma}^\star$. (That is, the weights of $\mathbf{\Gamma}^\star$ are the negatives of those of $\mathbf{\Gamma}$.)

Proof By the above construction, for any simple root α_j of $\tilde{\mathcal{L}}$, $\mathbf{\Gamma}^\star(ih_{\alpha_j}) = \{\mathbf{\Gamma}(ih_{\alpha_j})\}^\star = \{i\mathbf{\Gamma}(h_{\alpha_j})\}^\star = -i\{\mathbf{\Gamma}(h_{\alpha_j})\}^\star$. But Theorem III above implies that $\mathbf{\Gamma}(h_{\alpha_j})$ is a real matrix, so $\mathbf{\Gamma}^\star(ih_{\alpha_j}) = -i\mathbf{\Gamma}(h_{\alpha_j}) = -\mathbf{\Gamma}(ih_{\alpha_j})$, from which it follows that $\mathbf{\Gamma}^\star(h) = -\mathbf{\Gamma}(h)$ for *all* $h \in \mathcal{H}$. Consequently the weights of $\mathbf{\Gamma}^\star$ are the negatives of those of $\mathbf{\Gamma}$ and the multiplicity of $-\lambda$ in $\mathbf{\Gamma}^\star$ is equal to that of λ in $\mathbf{\Gamma}$.

One further simple property of representations and their weights is worth noting:

Theorem VII For *any* representation $\mathbf{\Gamma}$ of *any* semi-simple complex Lie algebra $\tilde{\mathcal{L}}$

$$\operatorname{tr} \mathbf{\Gamma}(a) = 0$$

for all $a \in \tilde{\mathcal{L}}$. In particular, for $a = h$ this implies that

$$\sum_\lambda m(\lambda)\lambda(h) = 0,$$

where the sum is over all the weights λ of $\mathbf{\Gamma}$. That is, on taking the multiplicities into account, the sum of the weights of *any* representation of $\tilde{\mathcal{L}}$ is *zero*.

Proof With the Weyl canonical basis of $\widetilde{\mathcal{L}}$ given in Chapter 3, Section 8, Equations (11.49) and (11.51) show that for *any* basis element a_p of $\widetilde{\mathcal{L}}$ there exist two basis elements a'_p and a''_p such that $a_p = \mu_p[a'_p, a''_p]$, where μ_p is some constant. Thus $\mathbf{\Gamma}(a_p) = \mu_p[\mathbf{\Gamma}(a'_p), \mathbf{\Gamma}(a''_p)]$. However, as $\mathrm{tr}\{\mathbf{\Gamma}(a'_p)\mathbf{\Gamma}(a''_p)\} = \mathrm{tr}\{\mathbf{\Gamma}(a''_p)\mathbf{\Gamma}(a'_p)\}$, then $\mathrm{tr}\,\mathbf{\Gamma}(a_p) = 0$, and hence $\mathrm{tr}\,\mathbf{\Gamma}(a) = 0$ for all $a \in \widetilde{\mathcal{L}}$.

With $a = h$, as the diagonal elements of $\mathbf{\Gamma}(h)$ are the quantities $\lambda(h)$, it follows immediately that $\sum_\lambda m(\lambda)\lambda(h) = 0$.

This result provides the final link in the proof of Theorem II of Chapter 4, Section 3:

Theorem VIII If $\mathcal{G}$ is a *non-compact* simple Lie group then $\mathcal{G}$ possesses *no* finite-dimensional unitary representations apart from the trivial representations in which $\mathbf{\Gamma}(T) = \mathbf{1}$ for all $T \in \mathcal{G}$.

Proof Suppose that $\mathcal{G}$ has a non-trivial d-dimensional unitary representation. Then the associated representation of $\mathcal{L}$, its real Lie algebra, consists of d-dimensional anti-Hermitian matrices, which, by the previous theorem, must be traceless. This representation must be faithful as $\mathcal{L}$ is simple, so $\mathcal{L}$ must be isomorphic to a subalgebra of $\mathrm{su}(d)$. As $\mathrm{su}(1)$ is trivial, d must be greater than 1. As $\mathrm{su}(d)$ is compact and semi-simple for $d \geq 2$, Theorem II of Chapter 11, Section 10, shows that $\mathcal{L}$ must be compact. This contradicts the conclusion of Theorem III of Chapter 11, Section 10, if $\mathcal{G}$ is non-compact, so the initial assumption that $\mathcal{G}$ possesses a non-trivial finite-dimensional unitary representation must be false.

3 The highest weight of a representation

In this section the very useful concept of the "highest" weight of a representation will be introduced. Each irreducible representation is uniquely and completely specified by its highest weight, all of its properties, such as its dimension and the other weights being easily deducible from it. Moreover, there is a straightforward procedure for constructing every possible highest weight.

It is convenient to define for the weights of a representation of $\widetilde{\mathcal{L}}$ a lexicographic ordering (see Chapter 11, Section 7) relative to the basis consisting of the simple roots $\alpha_1, \alpha_2, \ldots, \alpha_l$ of $\widetilde{\mathcal{L}}$. Then a weight λ is said to be "positive" if $\lambda = \sum_{j=1}^{l} \mu_j \alpha_j$ with the first non-vanishing component of the set $\{\mu_1, \mu_2, \ldots, \mu_l\}$ positive, Theorem III of the previous section having shown that all the members of this set are necessarily real. Further, if λ and λ' are two weights of a representation of $\widetilde{\mathcal{L}}$, one says that $\lambda > \lambda'$ if and only if $\lambda - \lambda' > 0$. (The second theorem of Chapter 11, Section 7, shows that a *root* α of $\widetilde{\mathcal{L}}$ is positive relative to $\beta_1, \beta_2, \ldots, \beta_l$ if and only if it is positive relative to $\alpha_1, \alpha_2, \ldots, \alpha_l$, so no confusion can arise from this new choice of a basis for lexicographic ordering.)

Definition *Highest weight Λ of a representation*
If Λ is a weight of a representation of $\widetilde{\mathcal{L}}$, such that $\Lambda > \lambda$ for every other weight λ, then Λ is said to be the "highest" weight of the representation.

Theorem I If Λ is the highest weight of an irreducible representation of a semi-simple complex Lie algebra $\widetilde{\mathcal{L}}$, then

(a) Λ is a *simple* weight (i.e. $m(\Lambda) = 1$); and

(b) *every* other weight λ of the representation has the form

$$\lambda = \Lambda - \sum_{j=1}^{l} q_j \alpha_j, \tag{12.9}$$

where $q_1, q_2, \ldots, q_l$ are a set of *non-negative integers.*

Proof See, for example, Appendix E, Section 12, of Cornwell (1984).

Definition *Fundamental weights of a semi-simple complex Lie algebra $\widetilde{\mathcal{L}}$*
The l "fundamental" weights $\Lambda_1(h), \Lambda_2(h), \ldots, \Lambda_l(h)$ of $\widetilde{\mathcal{L}}$ are the l linear functionals on $\mathcal{H}$ defined by

$$\Lambda_j(h) = \sum_{k=1}^{l} (\mathbf{A}^{-1})_{kj} \alpha_k(h) \tag{12.10}$$

for all $h \in \mathcal{H}$. (Here $\alpha_1, \alpha_2, \ldots, \alpha_l$ are the simple roots of $\widetilde{\mathcal{L}}$ and $\mathbf{A}$ is the Cartan matrix of $\widetilde{\mathcal{L}}$.)

It follows that

$$\frac{2\langle \Lambda_j, \alpha_k \rangle}{\langle \alpha_k, \alpha_k \rangle} = \delta_{jk}, \tag{12.11}$$

because, by Equations (11.45) and (12.10),

$$\begin{aligned} 2\langle \Lambda_j, \alpha_k \rangle / \langle \alpha_k, \alpha_k \rangle &= \sum_{p=1}^{l} 2(\mathbf{A}^{-1})_{pj} \langle \alpha_p, \alpha_k \rangle / \langle \alpha_k, \alpha_k \rangle \\ &= \sum_{p=1}^{l} (\mathbf{A}^{-1})_{pj} A_{kp} = \delta_{jk}. \end{aligned}$$

Conversely, Equation (12.11) implies Equation (12.10), so Equation (12.11) could equally well be taken as the definition of the fundamental weights.

It is worth noting that Equation (12.11) implies that

$$\Lambda_j(H_{\alpha_k}) = \delta_{jk},$$

for $j, k = 1, 2, \ldots, l$, where H_{α_k} is defined in Equation (11.21).

Theorem II For every irreducible representation of a semi-simple complex Lie algebra $\tilde{\mathcal{L}}$ the highest weight Λ can be written as

$$\Lambda = \sum_{j=1}^{l} n_j \Lambda_j, \tag{12.12}$$

where $\{n_1, n_2, \ldots, n_l\}$ is a set of *non-negative integers* and $\Lambda_1, \Lambda_2, \ldots, \Lambda_l$ are the fundamental weights of $\tilde{\mathcal{L}}$. Moreover, to *every* set of non-negative integers $\{n_1, n_2, \ldots, n_l\}$ there exists an irreducible representation of $\tilde{\mathcal{L}}$ with highest weight Λ given by Equation (12.12), and this representation is unique up to equivalence.

Proof See, for example, Chapter 15, Section 3, of Cornwell (1984) for a proof of the first part, for references to complete proofs, and a brief history.

Example I *The fundamental weights of the complexifications* $\tilde{\mathcal{L}} = A_1$ *and* A_2 *of* su(2) *and* su(3) *respectively*
From Example IV of Chapter 11, Section 7, for $\tilde{\mathcal{L}} = A_1$, $\mathbf{A}^{-1} = [1/2]$, while for $\tilde{\mathcal{L}} = A_2$

$$\mathbf{A}^{-1} = \begin{bmatrix} 2/3 & 1/3 \\ 1/3 & 2/3 \end{bmatrix}.$$

Thus the fundamental weight of $\tilde{\mathcal{L}} = A_1$ is

$$\Lambda_1 = (1/2)\alpha_1,$$

and the fundamental weights of $\tilde{\mathcal{L}} = A_2$ are

$$\left.\begin{aligned} \Lambda_1 &= (2/3)\alpha_1 + (1/3)\alpha_2, \\ \Lambda_2 &= (1/3)\alpha_1 + (2/3)\alpha_2. \end{aligned}\right\}$$

The irreducible representation of $\tilde{\mathcal{L}}$ with highest weight Λ specified by Equation (12.12) will be denoted by $\mathbf{\Gamma}(\{n_1, n_2, \ldots, n_l\})$. Its dimension d is given by the following remarkably simple formula, known as "Weyl's dimensionality formula".

Theorem III The dimension d of the irreducible representation of $\tilde{\mathcal{L}}$ with highest weight Λ is given by

$$d = \prod_{\alpha \in \Delta_+} \{\langle \Lambda + \delta, \alpha \rangle / \langle \delta, \alpha \rangle\}, \tag{12.13}$$

where $\delta = \frac{1}{2} \sum_{\alpha \in \Delta_+} \alpha$.

Proof Weyl (1925,1926a,b) deduced this result from his character formula. For details see, for example, Jacobson (1962), Samelson (1969), Humphreys (1972), or Varadarajan (1974).

Example II *Dimensions of the irreducible representations of the complexifications* $\widetilde{\mathcal{L}} = A_1$ *and* A_2 *of* su(2) *and* su(3) *respectively*
For $\widetilde{\mathcal{L}} = A_1$, as Δ_+ consists only of α_1, Equation (12.13) involves only one product, and shows that the dimension d of $\mathbf{\Gamma}(\{n_1\})$ is given by

$$d = n_1 + 1.$$

(Contact with the results of Chapter 10, Section 3, is obtained if n_1 is identified with $2j$, for $j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$).

For $\widetilde{\mathcal{L}} = A_2$, $\Delta_+ = \{\alpha_1, \alpha_2, \alpha_1 + \alpha_2\}$, so the dimension d of $\mathbf{\Gamma}(\{n_1, n_2\})$ is given by

$$d = \{n_1 + 1\}\{n_2 + 1\}\{(1/2)(n_1 + n_2) + 1\}. \tag{12.14}$$

In some very straightforward cases the other weights of an irreducible representation can be obtained from the highest weight by a simple application of Theorem IV of Section 2. For cases that are more complicated, but for which every weight is simple, Theorem V of Section 2 provides an elementary method for the deduction of the other weights. However, in general, some of the weights will not be simple, and a method is required for evaluating the multiplicities. "Freudenthal's recursion formula", which is stated in the next theorem, provides the necessary information. In this theorem the "level" q of a weight $\lambda = \Lambda - \sum_{j=1}^{l} q_j \alpha_j$ is defined to be $q = \sum_{j=1}^{l} q_j$. In particular, the highest weight Λ is of level zero and is the only weight of this level.

Theorem IV Consider an irreducible representation of $\widetilde{\mathcal{L}}$ that has highest weight Λ. Then the multiplicity $m(\lambda)$ of a possible weight $\lambda = \Lambda - \sum_{j=1}^{l} q_j \alpha_j$ (with $q_1, q_2, \ldots, q_l$ all non-negative integers) is given by

$$\{\langle \Lambda+\delta, \Lambda+\delta\rangle - \langle \lambda+\delta, \lambda+\delta\rangle\} m(\lambda) = 2 \sum_{\alpha \in \Delta_+} \sum_{k} m(\lambda+k\alpha)\langle \lambda+k\alpha, \alpha\rangle, \tag{12.15}$$

where the second sum on the right-hand side is only over those values of k for which $\lambda + k\alpha$ is a weight of the representation whose level is less than that of λ, and where $\delta = \frac{1}{2}\sum_{\alpha \in \Delta_+} \alpha$. In particular, if $m(\lambda) = 0$ then λ is *not* a weight of the representation.

Proof See Humphreys (1972) or Jacobson (1962).

As $m(\Lambda) = 1$, Freudenthal's recursion formula allows the multiplicities of the weights to be obtained first for level 1, then for level 2, and so on. For example, every level-1 weight has the form $\lambda = \Lambda - \alpha_j$, where α_j is some simple root. The only non-zero term on the right-hand side of Equation (12.15) occurs with $\alpha = \alpha_j$, and $k = 1$, and is $2m(\Lambda)\langle \Lambda, \alpha_j\rangle = 2\langle \Lambda, \alpha_j\rangle$. Similarly, every level-2 weight multiplicity is given by Equation (12.15) in terms of the multiplicities of weights of level 1 and 0, and so on.

It should be noted that if the linear functional $\lambda = \Lambda - \sum_{j=1}^{l} \alpha_j$ is not a weight, then Equation (12.15) gives $m(\lambda) = 0$. Consequently these formulae

provide a self-contained and exhaustive procedure for finding *all* the weights and their multiplicities, by simply investigating every linear functional of the form $\Lambda - \sum_{j=1}^{l} \alpha_j$, for every set of non-negative integers $\{q_1, q_2, \ldots, q_l\}$ for increasing values of $q = \sum_{j=1}^{l} q_j$, stopping when the sum of the multiplicities reaches the value d.

4 The irreducible representations of $\tilde{\mathcal{L}} = A_2$, the complexification of $\mathcal{L} = \mathbf{su(3)}$

As shown in Example I of Section 3, the fundamental weights of $\tilde{\mathcal{L}} = A_2$ are

$$\Lambda_1 = (2/3)\alpha_1 + (1/3)\alpha_2 \; \Lambda_2 = (1/3)\alpha_1 + (2/3)\alpha_2.$$

The corresponding two-component vectors are then

$$\boldsymbol{\Lambda}_1 = (2/3)\boldsymbol{\alpha}_1 + (1/3)\boldsymbol{\alpha}_2 \; \boldsymbol{\Lambda}_2 = (1/3)\boldsymbol{\alpha}_1 + (2/3)\boldsymbol{\alpha}_2,$$

from which it follows from Example II of Chapter 11, Section 6, that

$$\boldsymbol{\Lambda}_1 = (1/6)(\sqrt{3}, 1), \; \boldsymbol{\Lambda}_2 = (1/6)(0, 2).$$

Weyl's dimensionality formula implies that the dimension d of the irreducible representation $\boldsymbol{\Gamma}(\{n_1, n_2\})$ is given by Equation (12.14), that is,

$$d = \{n_1 + 1\}\{n_2 + 1\}\{(1/2)(n_1 + n_2) + 1\}. \tag{12.16}$$

If $n_1 \neq n_2$ a knowledge of the weights of $\boldsymbol{\Gamma}(\{n_1, n_2\})$ yields those of $\boldsymbol{\Gamma}(\{n_2, n_1\})$ immediately, for, if $\mu_1\alpha_1 + \mu_2\alpha_2$ is a weight of $\boldsymbol{\Gamma}(\{n_1, n_2\})$, then $\mu_1\alpha_2 + \mu_2\alpha_1$ is a weight of $\boldsymbol{\Gamma}(\{n_2, n_1\})$ with the same multiplicity. Moreover the weights of $\boldsymbol{\Gamma}(\{n_2, n_1\})$ are the negatives of those of $\boldsymbol{\Gamma}(\{n_1, n_2\})$. (This will be clear from inspection of the examples given below. A general proof can be found, for example, in Chapter 15, Section 4, of Cornwell (1984).)

In the elementary particle literature it is common to label each irreducible representation by its dimension d. When $n_1 \neq n_2$ Equation (12.16) shows that the irreducible representations $\boldsymbol{\Gamma}(\{n_1, n_2\})$ and $\boldsymbol{\Gamma}(\{n_2, n_1\})$ have the same dimension, one being the "complex conjugate" of the other in the sense of Section 2. In this case one representation is denoted by $\{d\}$ and the other by $\{d^\star\}$, the usual convention being

$$\boldsymbol{\Gamma}(\{n_1, n_2\}) = \begin{cases} \{d\} & \text{if } n_1 \geq n_2, \\ \{d^\star\} & \text{if } n_1 < n_2. \end{cases} \tag{12.17}$$

As shown in Example I of Chapter 11, Section 9, the Weyl group $\mathcal{W}$ of $\tilde{\mathcal{L}} = A_2$ consists of six elements S. As $S\lambda$ is a weight with the same multiplicity as λ for each $S \in \mathcal{W}$, the weights of an irreducible representation may be arranged in sets of six, three or one, the first occurring when $\boldsymbol{\lambda}$ is not

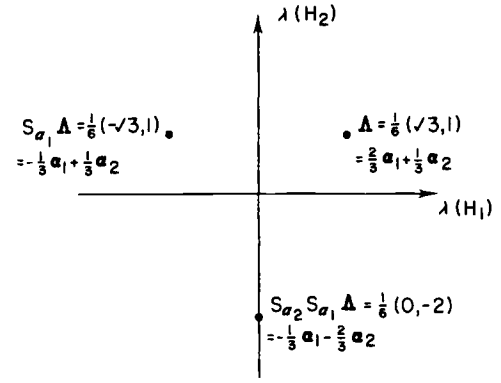

Figure 12.1: Weight diagram of the irreducible representation $\{3\}$ (specified by $n_1 = 1$, $n_2 = 0$) of $\widetilde{\mathcal{L}} = A_2$.

on a reflection line, the second when $\boldsymbol{\lambda}$ is on a reflection line and $\boldsymbol{\lambda} \neq \mathbf{0}$, and the third when $\boldsymbol{\lambda} = \mathbf{0}$.

The full sets of weights of the lower-dimensional irreducible representations of $\widetilde{\mathcal{L}} = A_2$ will now be examined.

(a) $\boldsymbol{\Gamma}(\{0,0\}) = \{1\}$:
With $n_1 = n_2 = 0$, Equation (12.16) gives $d = 1$. Consequently this irreducible representation has only one weight, namely the highest weight $\Lambda = 0$.

(b) $\boldsymbol{\Gamma}(\{1,0\}) = \{3\}$:
With $n_1 = 1$, $n_2 = 0$, Equation (12.16) gives $d = 3$. The highest weight is $\Lambda = \Lambda_1$, so $\boldsymbol{\Lambda} = \boldsymbol{\Lambda}_1 = \frac{1}{6}(\sqrt{3}, 1)$, which lies on a reflection line. Consequently this irreducible representation has two other simple weights $S_{\alpha_1}\Lambda$ and $S_{\alpha_2}S_{\alpha_1}\Lambda$, for which, by inspection of Figure 11.4, $S_{\alpha_1}\boldsymbol{\Lambda} = \frac{1}{6}(-\sqrt{3}, 1)$ and $S_{\alpha_2}S_{\alpha_1}\boldsymbol{\Lambda} = \frac{1}{6}(0, -2)$. This implies that $S_{\alpha_1}\boldsymbol{\Lambda} = \boldsymbol{\Lambda} - \boldsymbol{\alpha}_1$ and $S_{\alpha_2}S_{\alpha_1}\boldsymbol{\Lambda} = \boldsymbol{\Lambda} - (\boldsymbol{\alpha}_1 + \boldsymbol{\alpha}_2)$, so the weights of this irreducible representation are $\frac{2}{3}\boldsymbol{\alpha}_1 + \frac{1}{3}\boldsymbol{\alpha}_2$, $-\frac{1}{3}\boldsymbol{\alpha}_1 + \frac{1}{3}\boldsymbol{\alpha}_2$ and $-\frac{1}{3}\boldsymbol{\alpha}_1 - \frac{2}{3}\boldsymbol{\alpha}_2$. The weight diagram is given in Figure 12.1.

(c) $\boldsymbol{\Gamma}(\{0,1\}) = \{3^*\}$:
The weights of $\{3^*\}$ are $\frac{1}{3}\boldsymbol{\alpha}_1 + \frac{2}{3}\boldsymbol{\alpha}_2$ $(= \boldsymbol{\Lambda} = \boldsymbol{\Lambda}_2)$, $\frac{1}{3}\boldsymbol{\alpha}_1 - \frac{1}{3}\boldsymbol{\alpha}_2$ and $-\frac{2}{3}\boldsymbol{\alpha}_1 - \frac{1}{3}\boldsymbol{\alpha}_2$. The weight diagram is given in Figure 12.2.

(d) $\boldsymbol{\Gamma}(\{1,1\}) = \{8\}$:
With $n_1 = n_2 = 1$, Equation (12.16) gives $d = 8$. The highest weight is $\Lambda = \Lambda_1 + \Lambda_2 = \alpha_1 + \alpha_2$, so $\boldsymbol{\Lambda} = \boldsymbol{\alpha}_1 + \boldsymbol{\alpha}_2 = \frac{1}{6}(\sqrt{3}, 3)$. As this does not lie on a reflection line, there are five other simple weights obtained from it by Weyl reflections, which may be found by inspection using Figure 11.4. They are $\frac{1}{6}(-\sqrt{3}, 3)(= \boldsymbol{\alpha}_2)$, $\frac{1}{6}(\sqrt{3}, -3)(= -\boldsymbol{\alpha}_2)$,

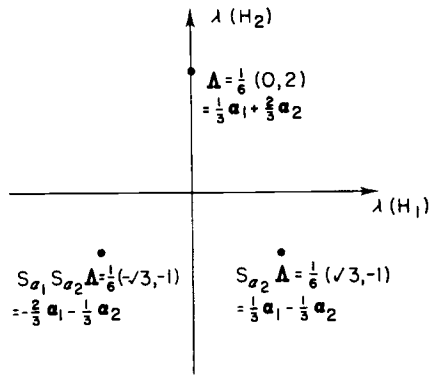

Figure 12.2: Weight diagram of the irreducible representation $\{3^*\}$ (specified by $n_1 = 0$, $n_2 = 1$) of $\widetilde{\mathcal{L}} = A_2$.

$\frac{1}{6}(-\sqrt{3}, -3)(= -\boldsymbol{\alpha}_1 - \boldsymbol{\alpha}_2)$, $\frac{1}{6}(2\sqrt{3}, 0)(= \boldsymbol{\alpha}_1)$ and $\frac{1}{6}(-2\sqrt{3}, 0)(= -\boldsymbol{\alpha}_1)$. As only six of the eight weights are thereby accounted for, all that can remain is a weight **0** of multiplicity 2. Clearly this representation is the adjoint representation. The weight diagram is given in Figure 12.3.

(e) $\boldsymbol{\Gamma}(\{2,0\}) = \{6\}$:
With $n_1 = 2$, $n_2 = 0$, Equation (12.16) gives $d = 6$. The highest weight is $\Lambda = 2\Lambda_1$, so $\boldsymbol{\Lambda} = 2\boldsymbol{\Lambda}_1 = \frac{1}{6}(2\sqrt{3}, 2)$, which lies on a reflection line. Exactly as for $\boldsymbol{\Gamma}(\{1,0\}) = \{3\}$, Weyl reflections then produce two more simple weights $\frac{1}{6}(-2\sqrt{3}, 2)$ and $\frac{1}{6}(0, -4)$. This leaves three other weights to be determined. However, for the α_1-string containing Λ, Equation (12.8) gives $p - q = 2\langle\Lambda, \alpha_1\rangle/\langle\alpha_1, \alpha_1\rangle = 2\{\frac{4}{3}\langle\alpha_1, \alpha_1\rangle + \frac{2}{3}\langle\alpha_2, \alpha_1\rangle\}/\langle\alpha_1, \alpha_1\rangle = \frac{4}{3}A_{11} + \frac{2}{3}A_{12} = 2$. As Λ is the highest weight, it follows that $q = 0$, implying $p = 2$, and giving as the α_1-string containing Λ the set $\{\Lambda, \Lambda - \alpha_1, \Lambda - 2\alpha_1\}$. But $\boldsymbol{\Lambda} - 2\boldsymbol{\alpha}_1 = \frac{1}{6}(-2\sqrt{3}, 2)$, which has been obtained already. However, $\boldsymbol{\Lambda} - \boldsymbol{\alpha}_1 = \frac{1}{6}(0, 2)$, which is new. Weyl reflections applied to this weight then produce $\frac{1}{6}(-\sqrt{3}, -1)$ and $\frac{1}{6}(\sqrt{3}, -1)$. Thus the weights are $\frac{4}{3}\alpha_1 + \frac{2}{3}\alpha_2$, $-\frac{2}{3}\alpha_1 + \frac{2}{3}\alpha_2$, $-\frac{2}{3}\alpha_1 - \frac{4}{3}\alpha_2$, $\frac{1}{3}\alpha_1 + \frac{2}{3}\alpha_2$, $\frac{1}{3}\alpha_1 - \frac{1}{3}\alpha_2$ and $-\frac{2}{3}\alpha_1 - \frac{1}{3}\alpha_2$, the weight diagram being given in Figure 12.4.

(f) $\boldsymbol{\Gamma}(\{0,2\}) = \{6^*\}$:
The weights of $\{6^*\}$ are the negatives of those of $\{6\}$ and are obtained by interchanging the coefficients of α_1 and α_2. The weight diagram is given in Figure 12.5.

(g) $\boldsymbol{\Gamma}(\{3,0\}) = \{10\}$:
The argument is essentially the same as for the $\{6\}$, producing the ten simple weights shown in Figure 12.6.

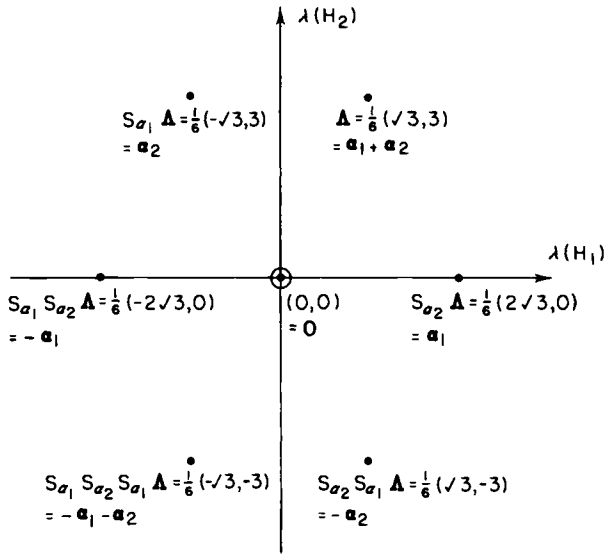

Figure 12.3: Weight diagram of the irreducible representation {8} (specified by $n_1 = n_2 = 1$) of $\widetilde{\mathcal{L}} = A_2$. (Here ⊙ indicates a weight of multiplicity 2.)

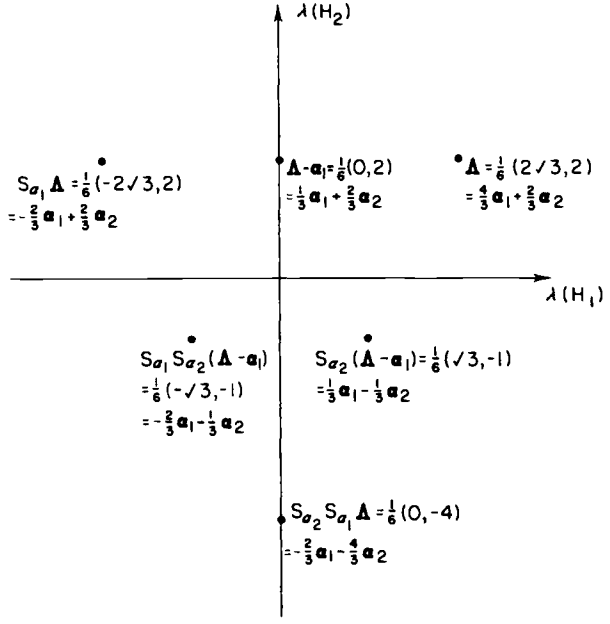

Figure 12.4: Weight diagram of the irreducible representation {6} (specified by $n_1 = 2$, $n_2 = 0$) of $\widetilde{\mathcal{L}} = A_2$.

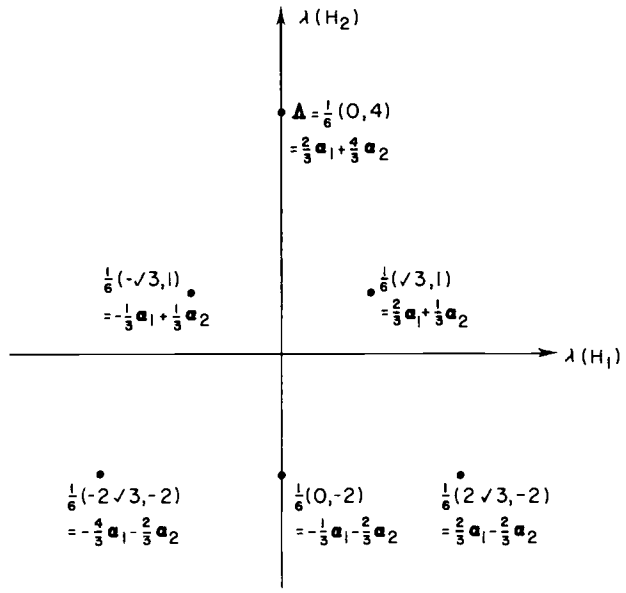

Figure 12.5: Weight diagram of the irreducible representation $\{6^*\}$ (specified by $n_1 = 0$, $n_2 = 2$) of $\widetilde{\mathcal{L}} = A_2$.

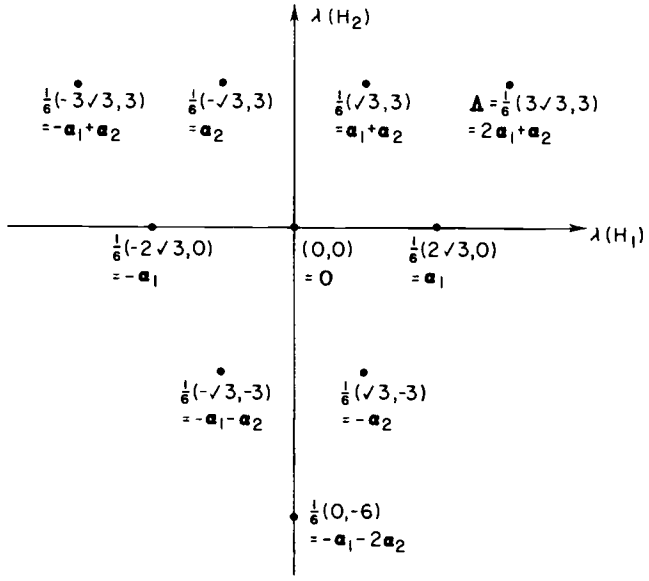

Figure 12.6: Weight diagram of the irreducible representation $\{10\}$ (specified by $n_1 = 3$, $n_2 = 0$) of $\widetilde{\mathcal{L}} = A_2$.

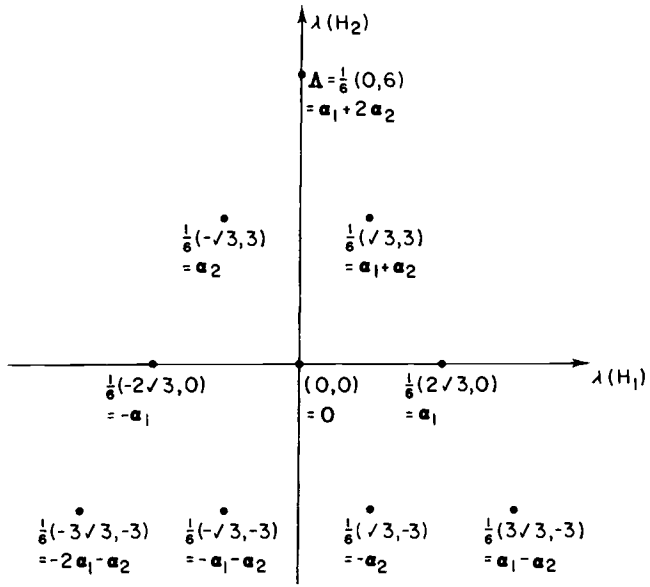

Figure 12.7: Weight diagram of the irreducible representation $\{10^*\}$ (specified by $n_1 = 0$, $n_2 = 3$) of $\widetilde{\mathcal{L}} = A_2$.

(h) $\mathbf{\Gamma}(\{0,3\}) = \{10^*\}$:
The weights of $\{10^*\}$ are the negatives of those of $\{10\}$ and are obtained by interchanging the coefficients of α_1 and α_2. The weight diagram is given in Figure 12.7.

As will become clear in Chapter 13, Section 3, the only higher-dimensional irreducible representations that are of interest in the su(3) symmetry scheme for hadrons are those for which $(n_1 - n_2)$ is divisible by three. Only one example will be considered in detail. Its mathematical interest lies in the fact that it provides the first case of a non-zero weight that is not simple.

(i) $\mathbf{\Gamma}(\{2,2\}) = \{27\}$:
The highest weight is $\Lambda = 2\Lambda_1 + 2\Lambda_2 = 2\alpha_1 + 2\alpha_2$. Application of Freudenthal's recursion formula (Equation (12.15)) shows that the weights of level 1 are $\Lambda - \alpha_1 (= \alpha_1 + 2\alpha_2)$ and $\Lambda - \alpha_2 (= 2\alpha_1 + \alpha_2)$, and that both are simple. Now consider the only possible weight of level 2, namely $\Lambda = \alpha_1 + \alpha_2$. As $\delta = \frac{1}{2}\{\alpha_1 + \alpha_2 + (\alpha_1 + \alpha_2)\} = \alpha_1 + \alpha_2$, Freudenthal's recursion formula (Equation (12.15)) gives

$$\begin{aligned}\{\langle 3(\alpha_1+\alpha_2), 3(\alpha_1+\alpha_2)\rangle - \langle 2(\alpha_1+\alpha_2), 2(\alpha_1+\alpha_2)\rangle\} m(\alpha_1+\alpha_2) \\ = 2\{m(2\alpha_1+2\alpha_2)\langle 2(\alpha_1+\alpha_2), \alpha_1+\alpha_2\rangle \\ + m(\alpha_1+2\alpha_2)\langle \alpha_1+2\alpha_2, \alpha_2\rangle + m(2\alpha_1+\alpha_2)\langle 2\alpha_1+\alpha_2, \alpha_1\rangle\},\end{aligned}$$

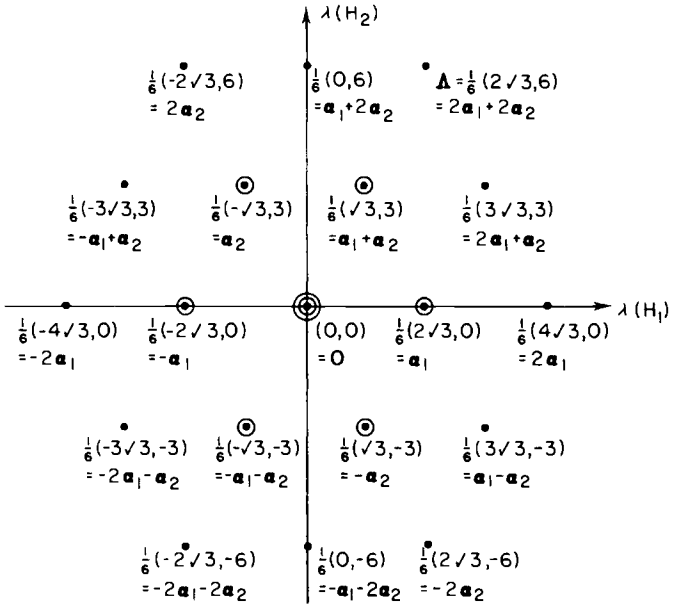

Figure 12.8: Weight diagram of the irreducible representation $\{27\}$ (specified by $n_1 = 2$, $n_2 = 2$) of $\widetilde{\mathcal{L}} = A_2$. (Here ⊙ and ◎ indicate weights of multiplicity 2 and 3 respectively.)

and, as $\langle \alpha_1, \alpha_1 \rangle = \frac{1}{3}$, $\langle \alpha_1, \alpha_2 \rangle = -\frac{1}{6}$ and $m(2\alpha_1 + 2\alpha_2) = m(\alpha_1 + 2\alpha_2) = m(2\alpha_1 + \alpha_2) = 1$, this gives $m(\alpha_1 + \alpha_2) = 2$. Repetition of this type of argument gives the weight diagram of Figure 12.8.

Some useful Clebsch-Gordan series for A_2 are:

$$\left.\begin{array}{lcl} \{3\} \otimes \{3^\star\} & \approx & \{8\} \oplus \{1\}, \\ \{3\} \otimes \{3\} \otimes \{3\} & \approx & \{10\} \oplus 2\{8\} \oplus \{1\}, \\ \{8\} \otimes \{8\} & \approx & \{27\} \oplus \{10\} \oplus \{10^\star\} \oplus 2\{8\} \oplus \{1\} \end{array}\right\} . \qquad (12.18)$$

(In the latter two Clebsch-Gordan series the expressions "$2\{8\}$" indicate that in each case the irreducible representation $\{8\}$ occurs with multiplicity 2. The Clebsch-Gordan coefficients for A_2 have been discussed in detail by de Swart (1963). For an introduction to the derivation of the Clebsch-Gordan series and coefficients for A_2 see, for example, Chapter 16, Sections 5 and 6, of Cornwell (1984).)

5 Casimir operators

In the analysis given in Chapter 10 of the representation theory of the su(2) (and so(3)) Lie algebras, a very important part was played by an operator A^2

defined in Equation (10.16). As noted in Equations (10.22), when written in the language of angular momentum theory, this is $(1/\hbar^2)$ times the operator J^2.

Casimir (1931) showed how a similar operator can be defined for *any* semi-simple Lie algebra. His prescription produced an operator of second order in the basis elements. This is appropriately called the "second-order Casimir operator" and is denoted by C_2. For $l > 1$ semi-simple Lie algebras possess other similar operators constructed using higher-order products. These will be called the "higher-order Casimir operators"

The basic properties of the second-order Casimir operator are summarized in the following theorem.

Theorem I Let $a_1, a_2, \ldots, a_n$ be a basis of a semi-simple Lie algebra $\mathcal{L}$ (either real or complex) and V be the carrier space of some representation $\mathbf{\Gamma}$ of $\mathcal{L}$ whose linear operators are $\Phi(a)$ $(a \in \mathcal{L})$. Then:

(a) The second-order Casimir operator C_2 specified by

$$C_2 = \sum_{p,q=1}^{n} (\mathbf{B}^{-1})_{pq} \Phi(a_p) \Phi(a_q) \tag{12.19}$$

is well defined and is independent of the choice of basis $a_1, a_2, \ldots, a_n$. (Here $\mathbf{B}$ is the $n \times n$ matrix with elements $B_{pq} = B(a_p, a_q)$.) In particular, for a basis of a complex (or compact real) semi-simple Lie algebra $\mathcal{L}$ such that $B(a_p, a_q) = -\delta_{pq}$

$$C_2 = -\sum_{p=1}^{n} \Phi(a_p)^2. \tag{12.20}$$

(b) C_2 commutes with $\Phi(a)$ for *all* $a \in \mathcal{L}$.

(c) If $\mathbf{\Gamma}$ is an irreducible representation of $\mathcal{L}$, then C_2 is a constant times the identity operator. If $\mathbf{\Gamma}$ has highest weight Λ, this constant will be written as $C_2(\Lambda)$. Then, for any $\psi \in V$,

$$C_2 \psi = C_2(\Lambda) \psi,$$

so that $C_2(\Lambda))$ may be described as the "eigenvalue of C_2 in the irreducible representation with highest weight Λ".

(d) This eigenvalue is given by the expression

$$C_2(\Lambda) = \langle \Lambda, \Lambda + 2\delta \rangle, \tag{12.21}$$

where

$$\delta = \frac{1}{2} \sum_{\alpha \in \Delta_+} \alpha. \tag{12.22}$$

(e) For the adjoint representation **ad**,

$$C_2(\Lambda) = 1.$$

Proof See, for example, Chapter 16, Section 2, of Cornwell (1984).

Example I *Second-order Casimir operator of* $\mathcal{L} = \mathrm{su}(2)$ $(= \mathrm{so}(3))$
With the operators A_1, A_2 and A_3 introduced in Chapter 10, Section 3, in terms of the basis a_1, a_2, a_3 of su(2) given in Equations (8.31), $A_p = -i\Phi(a_p)$ $(p = 1, 2, 3)$. However, with this basis $B(a_p, a_q) = -2\delta_{pq}$ (see Example I of Chapter 11, Section 2), so $(\mathbf{B}^{-1})_{pq} = -\frac{1}{2}\delta_{pq}$. Thus, from Equation (12.19),

$$C_2 = (A_1^2 + A_2^2 + A_3^2)/2 = A^2/2. \tag{12.23}$$

In terms of the angular momentum operator J^2, Equations (10.22) and (12.23) give

$$C_2 = (1/2\hbar^2)J^2. \tag{12.24}$$

For the irreducible representation with highest weight $\Lambda = n_1\Lambda_1 = \frac{1}{2}n_1\alpha_1$, as $\delta = \frac{1}{2}\alpha_1$ for $\mathcal{L} = A_1$, Equation (12.21) gives

$$\begin{aligned} C_2(\Lambda) &= \langle (1/2)n_1\alpha_1, (1/2)n_1\alpha_1 + \alpha_1\rangle = (1/4)n_1(n_1+2)\langle\alpha_1, \alpha_1\rangle \\ &= (1/8)n_1(n_1+2), \end{aligned}$$

as $\langle\alpha_1, \alpha_1\rangle = \frac{1}{2}$ (see Example I of Chapter 11, Section 4). Then, with $n_1 = 2j$ $(j = 0, \frac{1}{2}, 1, \ldots)$,

$$C_2(\Lambda) = j(j+1)/2,$$

so that the eigenvalues of A^2 are $j(j+1)$ (these being, of course, exactly the values found in Chapter 10, Section 3).

Example II *Second-order Casimir operator of* $\mathcal{L} = \mathrm{su}(3)$ *(and of* $\widetilde{\mathcal{L}} = A_2$*)*
For $\mathcal{L} = \mathrm{su}(3)$ (and $\widetilde{\mathcal{L}} = A_2$) $\delta = \alpha_1 + \alpha_2$ and $\Lambda_1 = \frac{2}{3}\alpha_1 + \frac{1}{3}\alpha_2$, $\Lambda_2 = \frac{1}{3}\alpha_1 + \frac{2}{3}\alpha_2$. Thus, for the irreducible representation $\mathbf{\Gamma}(\{n_1, n_2\})$ with highest weight $\Lambda = n_1\Lambda_1 + n_2\Lambda_2$,

$$\Lambda + 2\delta = \{(2/3)n_1 + (1/3)n_2 + 2\}\alpha_1 + \{(1/3)n_1 + (2/3)n_2 + 2\}\alpha_2.$$

Hence, by Equations (11.17) and (12.21),

$$C_2(\Lambda) = (n_1^2 + n_2^2 + n_1n_2 + 3n_1 + 3n_2)/9.$$

(As expected, $C_2(\Lambda) = 1$ for the adjoint representation $\mathbf{\Gamma}\{1, 1\}$.)

As an irreducible representation of a complex semi-simple Lie algebra $\widetilde{\mathcal{L}}$ is determined by its highest weight Λ, which itself depends on l (integer) parameters $n_1, n_2, \ldots, n_l$, one would *not* expect that specification of $C_2(\Lambda)$ would be sufficient to fix the irreducible representation. This expectation was

confirmed by Racah (1950, 1951), who showed that, if $\widetilde{\mathcal{L}}$ has rank l that is greater than 1, then $\widetilde{\mathcal{L}}$ possesses a set of higher-order Casimir operators whose eigenvalues do completely specify irreducible representations. See also Gruber and O'Raifeartaigh (1964), Okubo (1977), and Englefield and King (1980) for further work in this area.

Chapter 13

Symmetry schemes for the elementary particles

1 Leptons and hadrons

The starting point of all symmetry schemes for the elementary particles is the observation that there appear to be four fundamental interactions between these particles. These are, in decreasing order of strength:

(i) the strong interaction, first discussed in the context of the binding of the nucleons in the nucleus;

(ii) the electromagnetic interaction;

(iii) the weak interaction (which, for example, is responsible for beta decay);

(iv) the gravitational interaction.

(Recent developments suggest that these interactions may not be distinct, but may be manifestations of a single fundamental interaction.)

In terms of these four interactions it is possible to divide the observed particles into two major categories, the "leptons" (and "antileptons") which *never* experience strong interactions, and the "hadrons" (and "antihadrons") which, at least in some circumstances, interact through the strong interaction. In addition there are the "intermediate" particles that are the carriers of the interactions (of which the photon, $W^{\pm}$ and Z^0 have actually been observed at the time of writing). The category of *hadrons* can be further divided into two classes, those whose intrinsic spin j is an integer ($= 0, 1, 2, \ldots$) being called "mesons" and the others (for which $j = \frac{1}{2}, \frac{3}{2}, \ldots$) being referred to as "baryons". The "lepton number" and "baryon number" may then be defined for all the presently observed particles by

$$L = \begin{cases} 1, & \text{if the particle is a lepton,} \\ -1, & \text{if the particle is an antilepton,} \\ 0, & \text{for any other type of particle,} \end{cases}$$

and

$$B = \begin{cases} 1, & \text{if the particle is a baryon,} \\ -1, & \text{if the particle is an antibaryon,} \\ 0, & \text{for any other type of particle.} \end{cases}$$

2 The global internal symmetry group SU(2) and isotopic spin

The object of this section is to introduce the concept of isotopic spin and present the basic ideas in such a way that they are easily generalizable to other internal symmetries.

Consider first the case of the proton (p) and the neutron (n). Their rest masses m_p and m_n are almost identical ($m_pc^2 = 938.3$ MeV, $m_nc^2 = 939.6$ MeV), and their interactions with each other (that is p-p, p-n and n-n) are independent of how they are paired (provided that they are always coupled into the same state of total spin and parity). It is as though there is only one particle, the "nucleon" (N), which might exist in either of two states, one corresponding to the proton and the other to the neutron, these two states being distinguished only by an electromagnetic field. This is a similar situation to that of an atom in a state with orbital angular momentum l subjected to a small magnetic field $\mathbf{H}$. As noted in Chapter 10, Section 6, if all the effects of the electrons' spins are neglected (including degeneracies caused by them) then the energy eigenvalue of a state with angular momentum l is $(2l+1)$-fold degenerate in the absence of the field, but splits into $(2l+1)$ different values when the field is applied. Naturally one does not regard these as being $(2l+1)$ different atoms, but rather they are thought of as $(2l+1)$ different states of the same atom.

The correspondence between these two situations depends on the connection between energy and mass in the special theory of relativity. It leads to the proposal that the nucleon N should be assigned an "isotopic spin" I with value $\frac{1}{2}$ (this value being chosen so that $2I+1 = 2$, so that it can exist in $2I+1$ (=2) different states, one corresponding to the proton and one to the neutron. Further, it is suggested that in the absence of electromagnetic interactions (that is, in a universe with no electromagnetic interactions) the proton and the neutron would be identical, and each of their interactions, which are all "strong", would also be identical.

Developing this further, one can introduce three self-adjoint linear operators $\mathcal{I}_1$, $\mathcal{I}_2$ and $\mathcal{I}_3$ that satisfy the commutation relations

$$\left.\begin{aligned} [\mathcal{I}_1, \mathcal{I}_2] &= i\mathcal{I}_3, \\ [\mathcal{I}_2, \mathcal{I}_3] &= i\mathcal{I}_1, \\ [\mathcal{I}_3, \mathcal{I}_1] &= i\mathcal{I}_2. \end{aligned}\right\} \tag{13.1}$$

That is, more briefly,

$$[\mathcal{I}_p, \mathcal{I}_q] = i\sum_{r=1}^{3} \epsilon_{pqr}\mathcal{I}_r, \tag{13.2}$$

for $p, q = 1, 2, 3$. These are identical to the commutation relations in Equation (10.9). Indeed one can write, by analogy with Equation (10.7),

$$\mathcal{I}_p = -i\Phi(a_p), \tag{13.3}$$

(for $p = 1, 2, 3$), where a_1, a_2 and a_3 are basis elements of the real Lie algebra su(2). The analogy may be extended so that $\mathcal{I}_1$, $\mathcal{I}_2$ and $\mathcal{I}_3$ may be regarded as being operators corresponding to the measurement of the "components" of isotopic spin in three mutually perpendicular directions in an "isotopic spin space". Introducing the linear operator $\mathcal{I}^2$ by

$$\mathcal{I}^2 = (\mathcal{I}_1)^2 + (\mathcal{I}_2)^2 + (\mathcal{I}_3)^2 \tag{13.4}$$

(by analogy with Equation (10.16)), it is clear that all the properties of the operators A_1, A_2, A_3 and A^2 considered in Chapter 10, Section 3, apply equally to the operators $\mathcal{I}_1$, $\mathcal{I}_2$, $\mathcal{I}_3$ and $\mathcal{I}^2$. In particular, the operator $\mathcal{I}^2$ has eigenvalues of the form $I(I+1)$, where I takes one of the values $0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$. This quantity I is then regarded as the "isotopic spin", and the possible values of its "component in the third direction in isotopic spin space" associated with the operator $\mathcal{I}_3$ are given by the eigenvalue I_3 of $\mathcal{I}_3$, which assume any of the $(2I+1)$ values $I, I-1, \ldots, -I$. The simultaneous eigenvector of $\mathcal{I}^2$ and $\mathcal{I}_3$ with eigenvalues $I(I+1)$ and I_3 may be denoted (by analogy with Equations (10.23) and (10.24)) as $\psi^I_{I_3}$, so that

$$\left.\begin{array}{rcl} \mathcal{I}^2\psi^I_{I_3} & = & I(I+1)\psi^I_{I_3}, \\ \mathcal{I}_3\psi^I_{I_3} & = & I_3\psi^I_{I_3}. \end{array}\right\} \tag{13.5}$$

Indeed, for any element a of the su(2) Lie algebra spanned by the basis elements a_1, a_2 and a_3 of Equation (13.3),

$$\Phi(a)\psi^I_{I_3} = \sum_{I'_3=-I}^{I} D^I(a)_{I'_3 I_3}\psi^I_{I'_3}, \tag{13.6}$$

where $\mathbf{D}^I$ is the irreducible representation of su(2) introduced in Chapter 10, Section 3.

It may also be assumed that all these isotopic spin operators commute with all the operators corresponding to space-time transformations, so that the state vector of each hadron is the direct product of a function of space-time and one of the vectors $\psi^I_{I_3}$. Each value of I_3 corresponds to a particle, the set of $(2I+1)$ particles associated with a particular value I being said to form an "isotopic multiplet". It is implied from Equation (13.6) that the vectors $\psi^I_{I_3}$ form the basis of the $(2I+1)$-dimensional irreducible representation $\mathbf{D}^I$ of su(2). In the case of the nucleons, the proton is assigned the value $I_3 = \frac{1}{2}$ and the neutron the value $I_3 = -\frac{1}{2}$.

These considerations imply that all the particles in an isotopic multiplet must have the same intrinsic spin and parity, as well as the same baryon number (and other quantum numbers, such as strangeness and charm).

isotopic multiplet	B	Y	I	I_3	Q	particle
π, ρ	0	0	1	-1	-1	π^-, ρ^-
				0	0	π^0, ρ^0
				1	1	π^+, ρ^+
$K, K^\star$	0	1	$\frac{1}{2}$	$-\frac{1}{2}$	0	$K^0, K^{\star 0}$
				$\frac{1}{2}$	1	$K^+, K^{\star +}$
η, ϕ, ω	0	0	0	0	0	η^0, ϕ^0, ω^0
N	1	1	$\frac{1}{2}$	$-\frac{1}{2}$	0	n
				$\frac{1}{2}$	1	p
Δ	1	1	$\frac{3}{2}$	$-\frac{3}{2}$	-1	Δ^-
				$-\frac{1}{2}$	0	Δ^0
				$\frac{1}{2}$	1	Δ^+
				$\frac{3}{2}$	2	Δ^{++}
Λ	1	0	0	0	0	Λ^0
Σ	1	0	1	-1	-1	Σ^-
				0	0	Σ^0
				1	1	Σ^+
Ξ	1	-1	$\frac{1}{2}$	$-\frac{1}{2}$	-1	Ξ^-
				$\frac{1}{2}$	0	Ξ^0
Ω	1	-2	0	0	-1	Ω^-

Table 13.1: Isotopic spin, hypercharge and baryon number assignments of some of the most important hadrons.

It is assumed that *all hadrons* can be classified within this scheme. Historically, the earliest particles to be incorporated in this scheme after the nucleons were the three pions π^+, π^0 and π^-, which were assigned by to an isotopic multiplet with $I = 1$, the values of I_3 being 1, 0 and -1 respectively. For both the nucleons and the pions the electric charge Qe of the particle is given by

$$Q = I_3 + \frac{1}{2}B, \tag{13.7}$$

where B, the baryon number introduced in the previous section, has value 1 for the nucleons and 0 for the pions. In fact Equation (13.7) holds only for all non-strange and un-charmed hadrons, the generalization for strange hadrons being given later in Equation (13.9). A list of isotopic spin assignments for some of the most important hadrons is contained in Table 13.1.

The essential assumption underlying the above analysis is that the SU(2) group corresponding to the Lie algebra su(2) is the invariance group of the strong interaction Hamiltonian. This implies that this Hamiltonian and the corresponding T-matrix are irreducible tensor operators transforming as the one-dimensional identity irreducible representation. This enables predictions to be made of ratios of cross-sections and similar dynamical quantities using the Wigner-Eckart Theorem and the Clebsch-Gordan coefficients for su(2). (See, for example, Chapter 18, Section 2, of Cornwell (1984) for an introductory detailed analysis).

3 The global internal symmetry group SU(3) and strangeness

The present account of the su(3) symmetry scheme for hadrons is intended to introduce its most significant features and to emphasize the role of the group-theoretical and Lie-algebraic arguments developed in earlier chapters. There have been many long and detailed reviews of the su(3) scheme, and to these the reader is referred for more specific information on certain topics. The following list gives a selection of these: Behrends *et al.* (1962), Behrends (1968), Berestetskii (1965), Carruthers (1966), Charap *et al.* (1967), de Franceschi and Maiani (1965), de Swart (1963, 1965), Dyson (1966), Emmerson (1972), London (1964), Gatto (1964), Gell-Mann and Ne'eman (1964), Gourdin (1967), Kokkedee (1969), Lichtenberg (1978), Mathews (1967), Ne'eman (1965), O'Raifeartaigh (1968) and Smorodinsky (1965).

The concept of the strangeness quantum number was developed out of the "associated production" hypothesis of Pais (1952) to explain the observation that certain hadrons are created by strong interactions, but decay through the weak interaction (Gell-Mann 1953, Nakano and Nishijima 1953, Nishijima 1954, Gell-Mann and Pais 1955). The proposal was that every hadron possesses a "strangeness quantum number" S, which is assumed to be an integer, and that production or decay takes place through the strong interaction if and only if the quantity ΔS, defined by

$$\Delta S = \{\text{sum of initial values of } S\} - \{\text{sum of final values of } S\}, \tag{13.8}$$

is zero, that is, if and only if strangeness is additively conserved. The generalization of Equation (13.7) is given by the "Gell-Mann-Nishijima formula"

$$Q = I_3 + (1/2)B + (1/2)S, \tag{13.9}$$

(which is consistent with Equation (13.7), as nucleons and pions are assigned the value $S = 0$). This formula indicates that it is more convenient to work with the "hypercharge" Y defined by

$$Y = B + S, \tag{13.10}$$

in terms of which Equation (13.9) becomes

$$Q = I_3 + (1/2)Y. \tag{13.11}$$

Assuming that B is conserved, the selection rule for strong interactions is that they act if and only if

$$\Delta Y = 0. \tag{13.12}$$

Table 13.1 gives the assignment of hypercharge for some of the most important hadrons.

It is natural to assume that the possible values of Y are eigenvalues of a self-adjoint linear operator $\mathcal{Y}$. As all the particles in an isotopic multiplet are assumed to have the same value of Y, and as Y is assumed to be simultaneously measurable with I_3, it is necessary that

$$[\mathcal{Y}, \mathcal{I}_p] = 0 \tag{13.13}$$

for $p = 1, 2, 3$, implying that

$$[\mathcal{Y}, \mathcal{I}^2] = 0 \tag{13.14}$$

as well. Moreover, Y is assumed to be unchanged by space-time transformations.

As Y is an integer for all observed particles, it is reasonable to assume that $i\mathcal{Y}$ is the basis element of a real Lie algebra that is isomorphic to a u(1) real Lie algebra (the corresponding basis element of u(1) being $[i]$).) (As the unitary irreducible representations of the corresponding Lie group U(1) are all one-dimensional and are given by

$$\mathbf{\Gamma}_{\mathrm{U}(1)}([e^{ix}]) = [e^{ipx}],$$

where $p = 0, \pm 1, \pm 2, \ldots$, and where x is real, it follows that the corresponding irreducible representations of u(1) are such that

$$\mathbf{\Gamma}_{\mathrm{u}(1)}([i]) = [ip].$$

Then the eigenvalues of $\mathcal{Y}$ take the values $p = 0, \pm 1, \pm 2, \ldots$.) Consequently the set consisting of $i\mathcal{Y}$, $i\mathcal{I}_1$, $i\mathcal{I}_2$ and $i\mathcal{I}_3$ forms the basis of a u(1) $\oplus$ su(2) real Lie algebra (the commutation relations being Equations (13.1) and (13.13)). However, this alone does not imply any correlation between the eigenvalues of $\mathcal{Y}$ and $\mathcal{I}_3$. To obtain this it is necessary to make the further assumption that this u(1) $\oplus$ su(2) Lie algebra is the proper subalgebra of a larger real Lie algebra.

The natural candidates to consider are the rank-2 compact semi-simple real Lie algebras, because all their relevant properties are known. Being compact, all the finite-dimensional representations of their associated Lie groups are equivalent to unitary representations, which the isotopic spin arguments of the previous section suggest to be a desirable feature. A rank-2 algebra is appropriate because it can accommodate two mutually commuting operators

(corresponding to $\mathcal{Y}$ and $\mathcal{I}_3$) in its Cartan subalgebra. The non-simple candidate su(2) $\oplus$ su(2) can be eliminated because it would leave the values of $\mathcal{Y}$ and $\mathcal{I}_3$ unrelated, so the choice is narrowed to the rank-2 compact simple real Lie algebras. The analysis of Chapter 11 shows that there are only three non-isomorphic algebras with the required properties, namely su(3) (the compact real form of A_2), so(5) (which is the compact real form of B_2 and C_2, as these are isomorphic), and the compact real form of G_2. It is now clear that the scheme based on su(3) agrees well with experimental observation, and that this is not the case for the schemes based on the other algebras. Consequently the present account will be confined solely to the su(3) scheme. Even with su(3) selected as being the appropriate algebra, there still remains the question of the precise relationship of $\mathcal{Y}$ and $\mathcal{I}_3$ to the basis elements of the Cartan subalgebra of A_2. This is equivalent to the problem of assigning particles to multiplets, which was resolved by Gell-Mann (1961, 1962) and Ne'eman (1961), and which will be discussed shortly.

The basic philosophy of the su(3) scheme is that $\mathcal{Y}$ and $\mathcal{I}_3$ are members of the Cartan subalgebra of A_2, and their eigenvalues Y and I_3 are determined by the weights of the irreducible representations of A_2. The set of hadrons corresponding to a particular irreducible representation is said to form a "unitary multiplet" and the hadrons involved are assumed to be identical apart from their values of Y, I_3 and I, so that they all have the same spin, parity and baryon number. Moreover, it is assumed that in an ideal universe there is only one type of interaction, the strong interaction, and that all the particles in a unitary multiplet have exactly the same mass. At this point there is a problem, because it will become apparent that in the real world the particles in a unitary multiplet have masses that are only very roughly equal. The situation is quantitatively quite different from that in the isotopic spin scheme, where the masses within an isotopic multiplet differ by at most a few per cent, and where the difference can be attributed to the weaker electromagnetic interaction. It is clear that the considerable mass-splittings between isotopic multiplets in a unitary multiplet cannot be attributed to the electromagnetic interaction, so that it is necessary to make the assumption that there are two types of strong interaction. The weaker version, which will be called the "medium-strong interaction", is assumed to be responsible for these mass-splittings. The stronger version will still be referred to as "the" strong interaction

The first priority is to establish the relationship of $\mathcal{Y}$, $\mathcal{I}_1$, $\mathcal{I}_2$ and $\mathcal{I}_3$ to the basis elements h_{α_1}, h_{α_2}, e_{α_1}, $e_{-\alpha_1}$, e_{α_2}, $e_{-\alpha_2}$, $e_{\alpha_1+\alpha_2}$ and $e_{-(\alpha_1+\alpha_2)}$ of the Weyl canonical basis of A_2. The requirements are that:

(i) $\mathcal{I}_1, \mathcal{I}_2, \mathcal{I}_3$ satisfy the commutation relations in Equations (13.1);

(ii) $\mathcal{Y}$ satisfies the commutation relations in Equation (13.13); and

(iii) if any particle in a unitary multiplet has integral electric charge (that is, if Q is an integer), then *all* the particles in the multiplet must have integral electric charge.

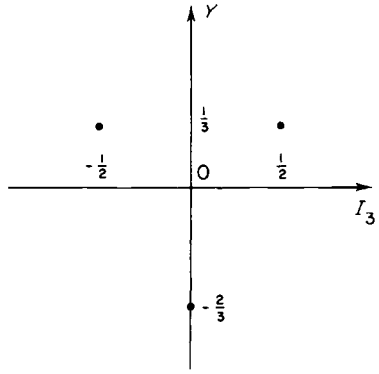

Figure 13.1: Values of I_3 and Y for the irreducible representation{3}.

These requirements lead to the assignments:

$$\left.\begin{aligned}
\mathcal{Y} &= \tfrac{1}{3}\Phi(H_{\alpha_1}) + \tfrac{2}{3}\Phi(H_{\alpha_2}) = 2\Phi(h_{\alpha_1}) + 4\Phi(h_{\alpha_2}) = 2\Phi(H_2), \\
\mathcal{I}_1 &= \tfrac{1}{2}\Phi(E_{\alpha_1}) + \tfrac{1}{2}\Phi(E_{-\alpha_1}) = \sqrt{3/2}\{\Phi(e_{\alpha_1}) - \Phi(e_{-\alpha_1})\}, \\
\mathcal{I}_2 &= -\tfrac{1}{2}i\Phi(E_{\alpha_1}) + \tfrac{1}{2}i\Phi(E_{-\alpha_1}) = -i\sqrt{3/2}\{\Phi(e_{\alpha_1}) + \Phi(e_{-\alpha_1})\}, \\
\mathcal{I}_3 &= \tfrac{1}{2}\Phi(H_{\alpha_1}) = 3\Phi(h_{\alpha_1}) = \sqrt{3}\Phi(H_1),
\end{aligned}\right\} \tag{13.15}$$

(where H_1 and H_2 are the ortho-normal basis elements of the Cartan subalgebra of A_2 of Example II of Chapter 11, Section 6). (The detailed argument that leads to Equations (13.15) may be found, for example, in Chapter 18, Section 3, of Cornwell (1984)).

The irreducible representations of A_2 were investigated in detail in Chapter 12, Section 4. For a weight

$$\lambda = \mu_1\alpha_1 + \mu_2\alpha_2, \tag{13.16}$$

the associated eigenvalues I_3 and Y of the operators $\mathcal{I}_3$ and $\mathcal{Y}$ are given by

$$\left.\begin{aligned}
I_3 &= \mu_1 - \tfrac{1}{2}\mu_2, \\
Y &= \mu_2.
\end{aligned}\right\} \tag{13.17}$$

The argument is simply that, by Equations (13.15) above,

$$I_3 = \lambda(3h_{\alpha_1}) = 3\{\mu_1\langle\alpha_1,\alpha_1\rangle + \mu_2\langle\alpha_1,\alpha_2\rangle\} = \mu_1 - (1/2)\mu_2,$$

and

$$\begin{aligned}
Y &= \lambda(2h_{\alpha_1} + 4h_{\alpha_2}) \\
&= \mu_1\{2\langle\alpha_1,\alpha_1\rangle + 4\langle\alpha_1,\alpha_2\rangle\} + \mu_2\{2\langle\alpha_1,\alpha_2\rangle + 4\langle\alpha_2,\alpha_2\rangle\} = \mu_2.
\end{aligned}$$

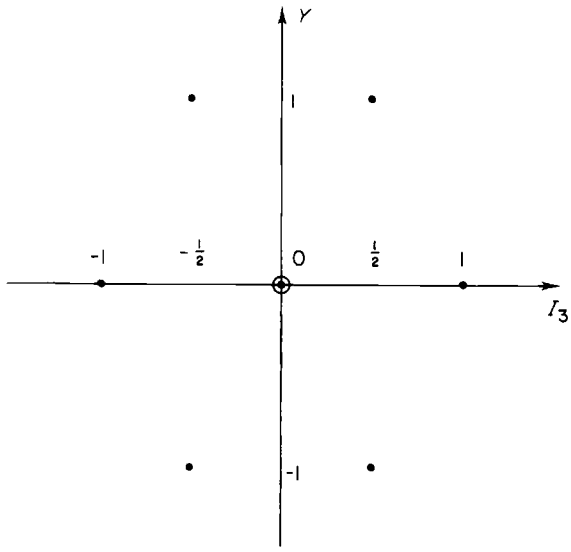

Figure 13.2: Values of I_3 and Y for the irreducible representation$\{8\}$.

The resulting pairs of eigenvalues I_3 and Y for the irreducible representations $\{3\}$, $\{8\}$, $\{6\}$ and $\{10\}$ can be read off Figures 12.1, 12.3, 12.4 and 12.6, and are displayed in Figures 13.1, 13.2, 13.3 and 13.4. For the representations $\{3^*\}$, $\{6^*\}$ and $\{10^*\}$ the values of I_3 and Y are the negatives of those of $\{3\}$, $\{6\}$ and $\{10\}$ respectively. By Equation (13.11) the corresponding values of the electric charge Qe are given by

$$Q = \mu_1. \tag{13.18}$$

The weight of multiplicity 2 of the irreducible representation $\{8\}$ may be thought of as being associated with two eigenvectors, one corresponding to the eigenvalues $I = 0$, $I_3 = 0$, $Y = 0$, and the other to $I = 1$, $I_3 = 0$, $Y = 0$.

The best-established non-trivial unitary multiplets are indicated in Figures 13.5, 13.6, 13.7 and 13.8. In each case the figure on the right hand side is the quantity mc^2, quoted in MeV, where m is the average rest mass of the corresponding isotopic multiplet. (The members of an isotopic multiplet necessarily lie in the same horizontal line in each of these figures.) To each of the baryon multiplets $\{8\}$ and $\{10\}$ there correspond antibaryons transforming as $\{8\}$ and $\{10^*\}$ respectively ($\{8\}$ being identical to its complex conjugate). At the time that this scheme was proposed all the particles of the baryon decuplet had already been observed, except for the Ω^-. The subsequent discovery of this particle with precisely the predicted quantum numbers (and a rest mass as predicted by the Gell-Mann-Okubo mass formula) was a triumph for the theory. In addition to the hadrons listed in the figures, there are a

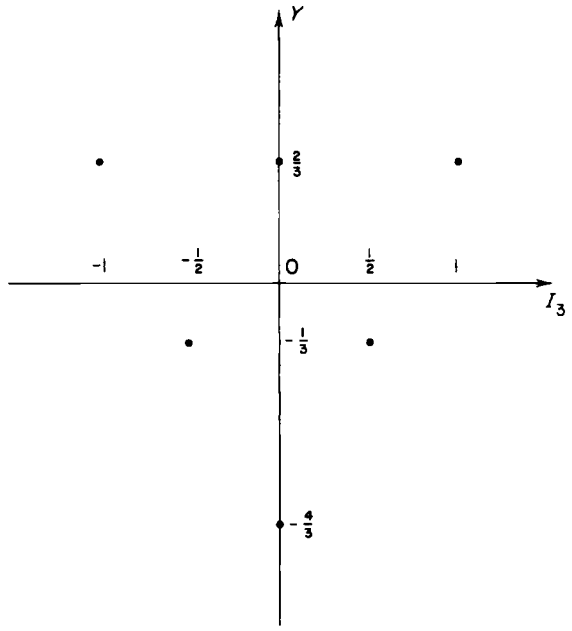

Figure 13.3: Values of I_3 and Y for the irreducible representation{6}.

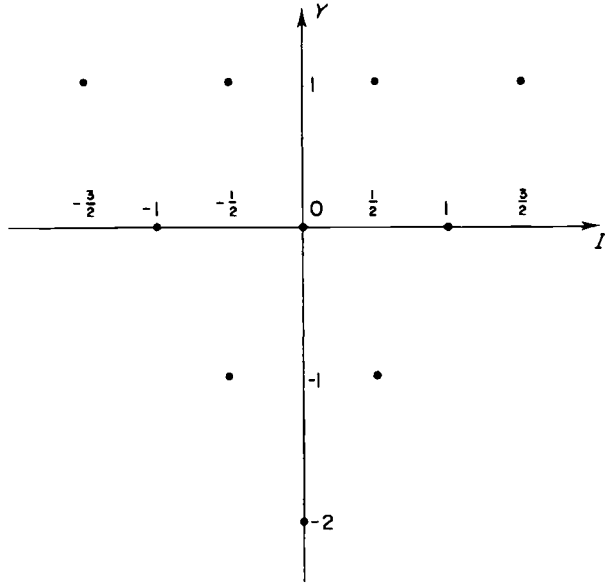

Figure 13.4: Values of I_3 and Y for the irreducible representation{10}.

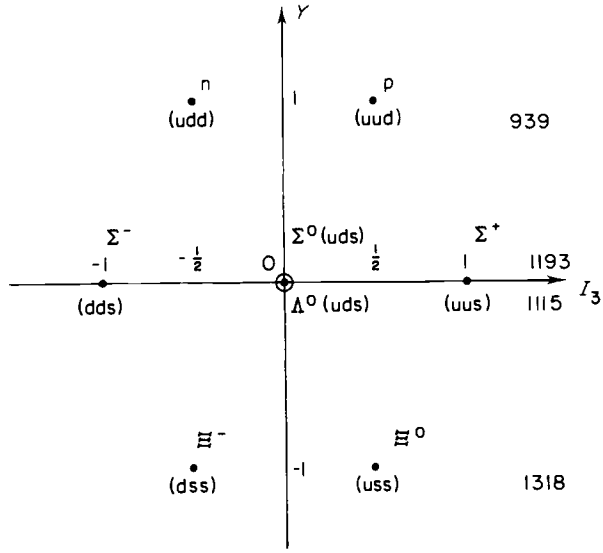

Figure 13.5: The baryon octet $\{8\}$ with $j = \frac{1}{2}$ and parity $+$. (The quark contents are in parentheses. The figures on the right hand side give mc^2 (in Mev), where m is the average mass of the isotopic multiplet to its left.)

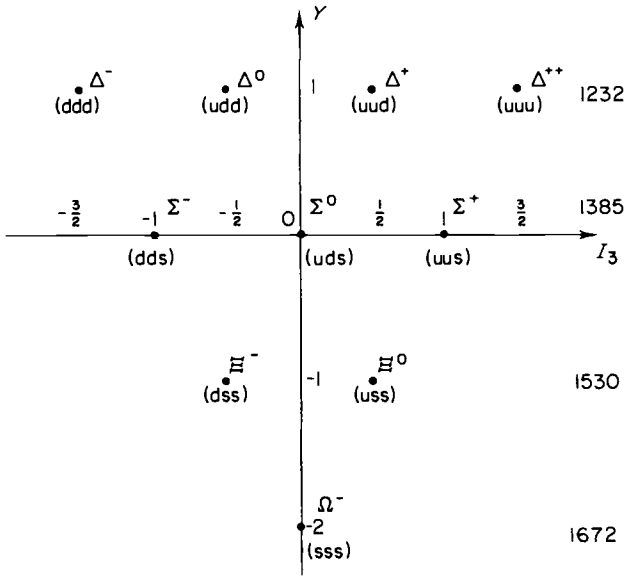

Figure 13.6: The baryon decuplet $\{10\}$ with $j = \frac{3}{2}$ and parity $+$. (The quark contents are in parentheses. The figures on the right hand side give mc^2 (in Mev), where m is the average mass of the isotopic multiplet to its left.)

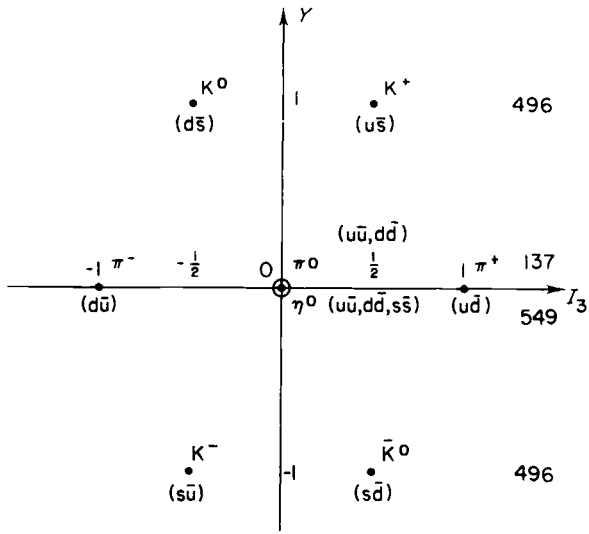

Figure 13.7: The meson octet $\{8\}$ with $j = 0$ and parity $-$. (The quark contents are in parentheses. The figures on the right hand side give mc^2 (in Mev), where m is the average mass of the isotopic multiplet to its left.)

number of singlets (belonging to the irreducible representation $\{1\}$).

One point that is immediately apparent from Figure 13.1 is that for the irreducible representation $\{3\}$ the values of Q are $\frac{2}{3}$, $-\frac{1}{3}$ and $-\frac{1}{3}$ i.e. *they are not integers.* This is actually a special case of the general result that the eigenvalues Q for the unitary multiplet belonging to the irreducible representation $\mathbf{\Gamma}(\{n_1, n_2\})$ are *integers if and only if* $(n_1 - n_2)/3$ *is an integer.* (The argument is that, by Equations (12.9) and (12.10), every weight λ in $\mathbf{\Gamma}(\{n_1, n_2\})$ is of the form

$$\lambda = n_1\Lambda_1 + n_2\Lambda_2 - q_1\alpha_1 - q_2\alpha_2 = \sum_{k=1}^{2}\{\sum_{j=1}^{2} n_j(\mathbf{A}^{-1})_{kj} - q_k\}\alpha_k \ ,$$

so that, from Equations (13.16) and (13.18),

$$Q = \sum_{j=1}^{2} n_j(\mathbf{A}^{-1})_{1j} - q_1 = (2/3)n_1 + (1/3)n_2 - q_1 = -(1/3)(n_1 - n_2) + n_1 - q_1.$$

As n_1, n_2, q_1, and q_2 are all integers, this expression is an integer if and only if $(n_1 - n_2)/3$ is an integer.)

The most fruitful proposal for dealing with this observation was made by Gell-Mann (1964) and Zweig (1964), and is that the particles corresponding to the irreducible representations $\{3\}$ and $\{3^*\}$ *do* exist, and are the basic constituents of all the observed hadrons. Gell-Mann (1964) called the particles of the $\{3\}$ "quarks", so that those of the $\{3^*\}$ become "antiquarks". The assumption is that the quarks have baryon number $B = \frac{1}{3}$ while the antiquarks

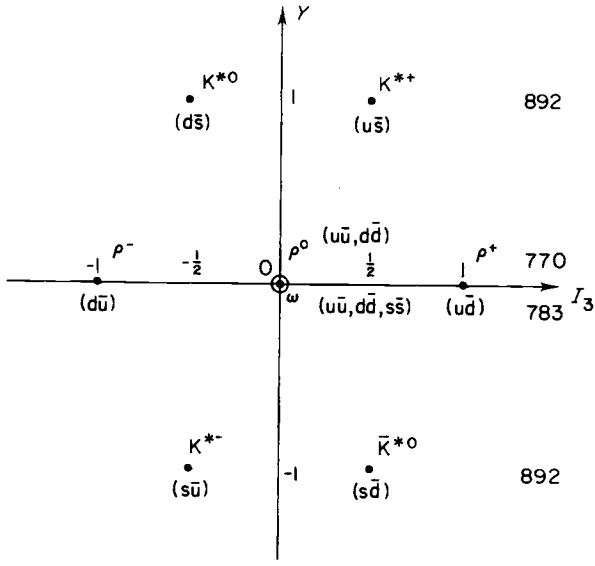

Figure 13.8: The meson octet $\{8\}$ with $j = 1$ and parity $-$. (The quark contents are in parentheses. The figures on the right hand side give mc^2 (in Mev), where m is the average mass of the isotopic multiplet to its left.)

correspond to $B = -\frac{1}{3}$. The three quarks are now usually called the u, d and s quarks (u corresponding to isotopic spin "up", d to isotopic spin "down", and s to non-zero strangeness), and the associated antiquarks are denoted by $\bar{u}$, $\bar{d}$ and $\bar{s}$. The properties of the quarks are summarized in Table 13.2.

In the simplest model the *mesons* are made of $q\bar{q}$ pairs (i.e. quark and antiquark pairs). As (10.38) shows that $\mathbf{D}^{1/2} \otimes \mathbf{D}^{1/2} \approx \mathbf{D}^1 \oplus \mathbf{D}^0$, two particles with intrinsic spin $\frac{1}{2}$ combine to produce composites with spin 1 and spin 0. Moreover, as noted in (12.18), for A_2 $\{3\} \otimes \{3^*\} \approx \{8\} \oplus \{1\}$, so that the $q\bar{q}$ pairs transform as the $\{8\}$ and the $\{1\}$. This explains very neatly the observation that there exist su(3) meson octets and singlets with both spin 1 and spin 0.

For *baryons* the simplest assumption is that each baryon consists of three quarks (and so each antibaryon consists of three antiquarks). As three particles with intrinsic spin $\frac{1}{2}$ couple to produce a composite with intrinsic spin $\frac{3}{2}$

quark	B	I	I_3	Y	S	Q
u	1/3	1/2	1/2	1/3	0	2/3
d	1/3	1/2	−1/2	1/3	0	−1/3
s	1/3	0	0	−2/3	−1	−1/3

Table 13.2: Quantum numbers of the quarks u, d and s.

or $\frac{1}{2}$ (because, by Equation (10.38)),

$$\begin{aligned}\mathbf{D}^{1/2} \otimes \mathbf{D}^{1/2} \otimes \mathbf{D}^{1/2} &\approx (\mathbf{D}^1 \oplus \mathbf{D}^0) \otimes \mathbf{D}^{1/2} \approx (\mathbf{D}^1 \otimes \mathbf{D}^{1/2}) \oplus (\mathbf{D}^0 \otimes \mathbf{D}^{1/2}) \\ &\approx (\mathbf{D}^{3/2} \oplus \mathbf{D}^{1/2}) \oplus \mathbf{D}^{1/2},\end{aligned}$$

and, as was noted in (12.18), for A_2 $\{3\} \otimes \{3\} \otimes \{3\} \approx \{10\} \oplus 2\{8\} \oplus \{1\}$, this provides a simple explanation of the existence of baryon octets of spin $\frac{1}{2}$ and baryon decuplets of spin $\frac{3}{2}$.

The quark contents suggested by the considerations are indicated in Figures 13.5, 13.6, 13.7 and 13.8.

When the unitary spin parts of the state vectors for the baryons are investigated along the lines indicated above for mesons, one very significant feature emerges. It can shown that the triple products of $\{3\}$ basis vectors that form basis vectors for the $\{10\}$ are *symmetric* with respect to the interchange of indices. Also, as $\mathbf{D}^{3/2}$ corresponds to the highest weight appearing in $\mathbf{D}^{1/2} \otimes \mathbf{D}^{1/2} \otimes \mathbf{D}^{1/2}$, the intrinsic spin part of the state vectors for the $\frac{3}{2}$ spin composites are *symmetric* products of the spin parts of the constituents. As the generalized Pauli Exclusion Principle states that fermion state vectors must be *antisymmetric* with respect to interchanges such as these, it follows that, if the only distinguishing labels for the quarks are those already introduced, then the orbital part of the three-quark wave functions for the spin-$\frac{3}{2}$ decuplet baryons must be *antisymmetric*. While this is not impossible, it is contrary to experience with ground state configurations in other systems. The dilemma can be avoided by making the further assumption that each of the three quarks u, d and s comes in *three* varieties that are distinguished by a further feature, which is called "colour". (It will be appreciated that this is purely a matter of terminology, and that it has nothing to do with "colour" in the normal sense of the word.) If each of the three quarks of a spin-$\frac{3}{2}$ decuplet has a different colour, then the internal symmetry part of the state vector is no longer symmetric, and so the problem with the orbital part does not arise. This idea forms the basis of the "SU(3) colour symmetry scheme" and thence of "quantum chromodynamics". In this scheme the strong interaction takes place through the exchange of 8 "gluons", which belong to the irreducible representation $\{8\}$ of the SU(3) colour group.

This introduction will be concluded by noting that it has proved very fruitful to extend the above considerations in various directions. The most straightforward generalization, from su(3) to su(4), produces a scheme with the additional quantum number "charm". The more sophisticated suggestion that symmetry breaking is "spontaneous" in origin gives rise to problems within "global" schemes (Goldstone 1961, Goldstone *et al.* 1962). However, as was shown by Higgs (1964a,b, 1966), when incorporated in a *gauge theory* (Yang and Mills 1954, and Shaw 1955) these difficulties not only disappear but permit mass generation of the intermediate particles, thereby allowing the construction of a unified theory of weak and electromagnetic interactions (c.f. Salam 1980, Weinberg 1980, and Glashow 1980), based on a $\mathrm{u}(1) \oplus \mathrm{su}(2)$ algebra.

APPENDICES

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Appendix A

Matrices

The object of this appendix is to give the definitions, notations and terminology for matrices that are used in this book, together with a brief but coherent account of their relevant properties.

1 Definitions

An $m \times n$ "matrix" $\mathbf{A}$ is defined as a rectangular array of mn elements A_{jk} $(1 \leq j \leq m, 1 \leq k \leq n)$, each of which is a real or complex number, arranged in m rows and n columns. That is

$$\mathbf{A} = \begin{bmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & & \vdots \\ A_{m1} & A_{m2} & \dots & A_{mn} \end{bmatrix}.$$

A matrix whose elements are all zero is called a "null matrix" or "zero matrix" and is denoted by $\mathbf{0}$.

When $m = n$, as is the case for most matrices encountered in this book, the matrix is said to be "square". In this case the elements A_{jk} with $j = k$ are called the "diagonal" elements, while those with $j < k$ are referred to as being in the "upper off-diagonal" positions. If $A_{jk} = 0$ for $j \neq k$ then $\mathbf{A}$ is said to be a "diagonal matrix". the most important example is the "unit matrix" $\mathbf{1}$, which is defined by

$$(\mathbf{1})_{jk} = \delta_{jk} = \begin{cases} 1, \text{ if } j = k, \\ 0, \text{ if } j \neq k, \end{cases}$$

δ_{jk} being the Kronecker delta symbol. (The dimension of $\mathbf{1}$ is usually clear from its context, but when this is not so the $m \times m$ unit matrix will be denoted by $\mathbf{1}_m$.)

The "sum" of two $m \times n$ matrices $\mathbf{A}$ and $\mathbf{B}$ is defined to be another $m \times n$ matrix $\mathbf{A} + \mathbf{B}$ such that $(\mathbf{A} + \mathbf{B})_{jk} = A_{jk} + B_{jk}$ $(1 \leq j \leq m, 1 \leq k \leq n)$.

Similarly, the "scalar product" of an $m \times n$ matrix $\mathbf{A}$ with a real or complex number λ is an $m \times n$ matrix $\lambda\mathbf{A}$ defined such that $(\lambda\mathbf{A})_{jk} = \lambda A_{jk}$ $(1 \leq j \leq m, 1 \leq k \leq n)$. The "matrix product" of an $m \times n$ matrix $\mathbf{A}$ and an $n \times p$ matrix $\mathbf{B}$ is defined as an $m \times p$ matrix $\mathbf{AB}$ whose elements are given by

$$(\mathbf{AB})_{jl} = \sum_{k=1}^{n} A_{jk} B_{kl}. \tag{A.1}$$

When $m = n = p$, both $\mathbf{AB}$ and $\mathbf{BA}$ exist and have the same dimensions, but even so, in general, $\mathbf{AB} \neq \mathbf{BA}$. However, if $\mathbf{A}$ and $\mathbf{B}$ are both diagonal matrices, then necessarily $\mathbf{AB} = \mathbf{BA}$. Of course, for any $m \times n$ matrix $\mathbf{A}$, $\mathbf{A1} = \mathbf{1A} = \mathbf{A}$.

The "transpose" $\widetilde{\mathbf{A}}$ of an $m \times n$ matrix $\mathbf{A}$ is defined to be the $n \times m$ matrix whose elements are given by $(\widetilde{\mathbf{A}})_{jk} = A_{kj}$, so that if $\mathbf{C} = \mathbf{AB}$ then $\widetilde{\mathbf{C}} = \widetilde{\mathbf{B}}\widetilde{\mathbf{A}}$. The "complex conjugate" $\mathbf{A}^\star$ of $\mathbf{A}$ is defined as the $m \times n$ matrix such that $(\mathbf{A}^\star)_{jk} = (A_{jk})^\star$, the $\star$ here denoting complex conjugation. Combining these concepts gives the "Hermitian adjoint" $\mathbf{A}^\dagger$ of $\mathbf{A}$, which is the $n \times m$ matrix defined by $\mathbf{A}^\dagger = (\widetilde{\mathbf{A}})^\star$. (In the mathematical literature this $\mathbf{A}^\dagger$ is often referred to as the "associate" of $\mathbf{A}$, the term "adjoint" being reserved for another matrix.)

The "determinant" $\det \mathbf{A}$ of an $m \times m$ matrix $\mathbf{A}$ is the real or complex number defined by $\det \mathbf{A} = \sum(-1)^p A_{1c_1} A_{2c_2} \ldots A_{mc_m}$, where $(c_1, c_2, \ldots, c_m)$ is a permutation of $(1, 2, \ldots, m)$, p being the number of transpositions required to bring $(c_1, c_2, \ldots, c_m)$ to the "natural" order $(1, 2, \ldots, m)$, and the sum is over all such permutations. Then $\det \mathbf{1} = 1$, and

$$\det \widetilde{\mathbf{A}} = \det \mathbf{A}, \tag{A.2}$$

$$\det \mathbf{A}^\star = (\det \mathbf{A})^\star, \tag{A.3}$$

$$\det(\mathbf{AB}) = (\det \mathbf{A})(\det \mathbf{B}), \tag{A.4}$$

Moreover, if $\mathbf{B}$ is a matrix obtained from $\mathbf{A}$ by interchanging all the elements of a pair of rows (or a pair of columns), then $\det \mathbf{B} = -\det \mathbf{A}$.

The "inverse" $\mathbf{A}^{-1}$ of an $m \times m$ matrix $\mathbf{A}$ is defined as the $m \times m$ matrix such that $\mathbf{A}^{-1}\mathbf{A} = \mathbf{A}\mathbf{A}^{-1} = \mathbf{1}$. $\mathbf{A}^{-1}$ exists if and only if $\det \mathbf{A} \neq 0$, in which case $\mathbf{A}$ is described as being "non-singular". If $\mathbf{A}$ and $\mathbf{B}$ are two non-singular $m \times m$ matrices, then $(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}$.

Table A.1 gives the definitions of a number of important special types of matrix. It should be noted that a matrix that is both real and symmetric is necessarily Hermitian, and a matrix that is both real and orthogonal is necessarily unitary. For an *orthogonal* matrix $\mathbf{A}$, as $\widetilde{\mathbf{A}}\mathbf{A} = \mathbf{1}$, Equations (A.2) and (A.4) imply that $(\det \mathbf{A})^2 = 1$, so that

$$\det \mathbf{A} = +1 \text{ or } -1. \tag{A.5}$$

Similarly, for a *unitary* matrix $\mathbf{A}$, as $\mathbf{A}^\dagger\mathbf{A} = \mathbf{1}$, Equations (A.2), (A.3) and (A.4) imply that $|\det \mathbf{A}|^2 = 1$, so that

$$\det \mathbf{A} = \exp(i\alpha), \tag{A.6}$$

Description of matrix	*Defining property*
symmetric	$\widetilde{\mathbf{A}} = \mathbf{A}$
antisymmetric (or skew-symmetric)	$\widetilde{\mathbf{A}} = -\mathbf{A}$
real	$\mathbf{A}^* = \mathbf{A}$
orthogonal	$\widetilde{\mathbf{A}} = \mathbf{A}^{-1}$
Hermitian (or self-adjoint)	$\mathbf{A}^\dagger = \mathbf{A}$
anti-Hermitian	$\mathbf{A}^\dagger = -\mathbf{A}$
unitary	$\mathbf{A}^\dagger = \mathbf{A}^{-1}$
anti-unitary	$\mathbf{A}^\dagger = -\mathbf{A}^{-1}$

Table A.1: Definitions of special types of matrix.

where α is some real number.

The "trace" $\mathrm{tr}\mathbf{A}$ of an $m \times m$ matrix $\mathbf{A}$ is defined by $\mathrm{tr}\mathbf{A} = \sum_{j=1}^{m} A_{jj}$, that is, it is the sum of the diagonal elements of $\mathbf{A}$. If $\mathbf{A}$ and $\mathbf{B}$ are any two $m \times m$ matrices, it follows immediately from Equation (A.1) that $\mathrm{tr}(\mathbf{AB}) = \mathrm{tr}(\mathbf{BA})$. Also $\mathrm{tr}(\mathbf{A}+\mathbf{B}) = \mathrm{tr}\,\mathbf{A} + \mathrm{tr}\,\mathbf{B}$, and, for any complex number α, $\mathrm{tr}(\alpha\mathbf{A}) = \alpha(\mathrm{tr}\,\mathbf{A})$. Moreover, if $\mathbf{A}, \mathbf{B}, \mathbf{C}$ are any three $m \times m$ matrices, Equation (A.1) gives $\mathrm{tr}(\mathbf{ABC}) = \mathrm{tr}(\mathbf{BCA}) = \mathrm{tr}(\mathbf{CAB})$. If $\mathrm{tr}\,\mathbf{A} = 0$, then $\mathbf{A}$ is said to be "traceless". If $\mathbf{A}$ and $\mathbf{A}'$ are $m \times m$ matrices related by a so-called "similarity transformation" $\mathbf{A}' = \mathbf{S}^{-1}\mathbf{AS}$, where $\mathbf{S}$ is any $m \times m$ non-singular matrix, then $\mathrm{tr}\,\mathbf{A}' = \mathrm{tr}\,\mathbf{A}$.

A matrix may be "partitioned" into submatrices by inserting dividing lines between arbitrarily chosen adjacent pairs of rows and columns. For example,

$$\mathbf{A} = \left[\begin{array}{c|ccc} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ \hline A_{31} & A_{32} & A_{33} & A_{34} \end{array}\right] = \left[\begin{array}{c|c|c} \mathbf{A}^{11} & \mathbf{A}^{12} & \mathbf{A}^{13} \\ \hline \mathbf{A}^{21} & \mathbf{A}^{22} & \mathbf{A}^{23} \end{array}\right]$$

is a partitioning of a 3×4 matrix $\mathbf{A}$ into six submatrices $\mathbf{A}^{jk}$, defined by

$$\mathbf{A}^{11} = \begin{bmatrix} A_{11} \\ A_{21} \end{bmatrix}, \quad \mathbf{A}^{12} = \begin{bmatrix} A_{12} & A_{13} \\ A_{22} & A_{23} \end{bmatrix}, \quad \mathbf{A}^{13} = \begin{bmatrix} A_{14} \\ A_{24} \end{bmatrix},$$

$$\mathbf{A}^{21} = [A_{31}], \quad \mathbf{A}^{22} = [A_{32}\ A_{33}], \quad \mathbf{A}^{23} = [A_{34}].$$

In terms of submatrices, the matrix product $\mathbf{C} = \mathbf{AB}$ of an $m \times n$ matrix $\mathbf{A}$ with an $n \times p$ matrix $\mathbf{B}$ has a remarkably simple property, provided that the "column" partitioning of $\mathbf{A}$ is chosen to be the same as the "row" partitioning of $\mathbf{B}$. Explicitly, if $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ are partitioned into st submatrices $\mathbf{A}^{jk}$, tu submatrices $\mathbf{B}^{kl}$ and su submatrices $\mathbf{C}^{jl}$ respectively, where $1 \le j \le s \le m$, $1 \le k \le t \le n$, $1 \le l \le u \le p$, and where $\mathbf{A}^{jk}$, $\mathbf{B}^{kl}$ and $\mathbf{C}^{jl}$ have dimensions $m_j \times n_k$, $n_k \times p_l$ and $m_j \times p_l$ respectively (where $\sum_{j=1}^{s} m_j = m$, $\sum_{k=1}^{t} n_k = n$, and $\sum_{l=1}^{u} p_l = p$, then

$$\mathbf{C}^{jl} = \sum_{k=1}^{t} \mathbf{A}^{jk}\mathbf{B}^{kl}. \tag{A.7}$$

There is a striking similarity of form with Equation (A.1). It is as though the submatrices $\mathbf{A}^{jk}$, $\mathbf{B}^{kl}$ and $\mathbf{C}^{jl}$ can be regarded as being matrix elements, but with the product of $\mathbf{A}^{jk}$ and $\mathbf{B}^{kl}$ being given by Equation (A.1). For clarity, the various submatrices have been distinguished here by superscripts. However, it is sometimes convenient to use subscripts instead, as, for example, in Chapter 4, Section 4. Moreover, the dividing lines will be omitted when there is no possibility of confusion, so that for the above example

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}^{11} & \mathbf{A}^{12} & \mathbf{A}^{13} \\ \mathbf{A}^{21} & \mathbf{A}^{22} & \mathbf{A}^{23} \end{bmatrix}.$$

The "direct product" (or "Kronecker product") of an $m \times m$ matrix $\mathbf{A}$ and an $n \times n$ matrix $\mathbf{B}$ is defined to be an $mn \times mn$ matrix $\mathbf{A} \otimes \mathbf{B}$, whose rows and columns are each labelled by a *pair* of indices in such a way that

$$(\mathbf{A} \otimes \mathbf{B})_{js,kt} = A_{jk}B_{st} \quad (\text{for } 1 \leq j,k \leq m \text{ and } 1 \leq s,t \leq n). \tag{A.8}$$

In order to express such matrices in the usual form in which rows and columns are each labelled by a single index it is necessary to put the set of mn pairs (j,s) $(1 \leq j \leq m;\ 1 \leq s \leq n)$ into one-to-one correspondence with a set of mn integers p $(1 \leq p \leq mn)$, with an identical correspondence between the pairs (k,t) and a set of integers q. The most convenient choice is $p = n(j-1)+s$, $q = n(k-1)+t$. With this prescription, the matrix $\mathbf{A} \otimes \mathbf{B}$ for $m = 2$ and $n = 2$ would be displayed as

$$\begin{bmatrix} (\mathbf{A}\otimes\mathbf{B})_{11,11} & (\mathbf{A}\otimes\mathbf{B})_{11,12} & (\mathbf{A}\otimes\mathbf{B})_{11,21} & (\mathbf{A}\otimes\mathbf{B})_{11,22} \\ (\mathbf{A}\otimes\mathbf{B})_{12,11} & (\mathbf{A}\otimes\mathbf{B})_{12,12} & (\mathbf{A}\otimes\mathbf{B})_{12,21} & (\mathbf{A}\otimes\mathbf{B})_{12,22} \\ (\mathbf{A}\otimes\mathbf{B})_{21,11} & (\mathbf{A}\otimes\mathbf{B})_{21,12} & (\mathbf{A}\otimes\mathbf{B})_{21,21} & (\mathbf{A}\otimes\mathbf{B})_{21,22} \\ (\mathbf{A}\otimes\mathbf{B})_{22,11} & (\mathbf{A}\otimes\mathbf{B})_{22,12} & (\mathbf{A}\otimes\mathbf{B})_{22,21} & (\mathbf{A}\otimes\mathbf{B})_{22,22} \end{bmatrix}.$$

Clearly, the diagonal elements of $\mathbf{A} \otimes \mathbf{B}$ in the pair-labelling scheme are those for which $j = k$ *and* $s = t$. If $\mathbf{A}$ and $\mathbf{B}$ are both diagonal, then $\mathbf{A} \otimes \mathbf{B}$ is also diagonal (for if $A_{jk} = a_j\delta_{jk}$ and $B_{st} = b_s\delta_{st}$, then $(\mathbf{A} \otimes \mathbf{B})_{js,kt} = a_jb_s\delta_{jk}\delta_{st}$).

If $\mathbf{A}$ and $\mathbf{A}'$ are both $m \times m$ matrices and $\mathbf{B}$ and $\mathbf{B}'$ are both $n \times n$ matrices, then

$$(\mathbf{A} \otimes \mathbf{B})(\mathbf{A}' \otimes \mathbf{B}') = (\mathbf{A}\mathbf{A}') \otimes (\mathbf{B}\mathbf{B}'), \tag{A.9}$$

where all products other than those indicated by the symbol $\otimes$ are ordinary matrix products (as defined in Equation (A.1)). The proof of Equation (A.9) is straightforward, for the (js,kt) element of the right-hand side is

$$(\mathbf{A}\mathbf{A}')_{jk}(\mathbf{B}\mathbf{B}')_{st} = \sum_{l=1}^{m}\sum_{u=1}^{n} A_{jl}A'_{lk}B_{su}B'_{ut},$$

while the (js,kt) element of the left-hand side is

$$\sum_{l=1}^{m}\sum_{u=1}^{n}(\mathbf{A}\otimes\mathbf{B})_{js,lu}(\mathbf{A}'\otimes\mathbf{B}')_{lu,kt} = \sum_{l=1}^{m}\sum_{u=1}^{n} A_{jl}B_{su}A'_{lk}B'_{ut}.$$

Finally, if $\mathbf{A}$ and $\mathbf{B}$ are both unitary, then $\mathbf{A} \otimes \mathbf{B}$ is also unitary. (It follows directly from Equation (A.8) that $(\mathbf{A} \otimes \mathbf{B})^\dagger = \mathbf{A}^\dagger \otimes \mathbf{B}^\dagger$, and, as $\mathbf{A}^\dagger\mathbf{A} = \mathbf{A}\mathbf{A}^\dagger = \mathbf{1}_m$, $\mathbf{B}^\dagger\mathbf{B} = \mathbf{B}\mathbf{B}^\dagger = \mathbf{1}_n$ and $\mathbf{1}_m \otimes \mathbf{1}_n = \mathbf{1}_{m+n}$, the unitary property of $\mathbf{A} \otimes \mathbf{B}$ is an immediate consequence of Equation (A.9).)

2 Eigenvalues and eigenvectors

If $\mathbf{A}$ is an $m \times m$ matrix and λ is a real or complex number which, together with an $m \times 1$ "column" matrix $\mathbf{c}$ ($\mathbf{c} \neq \mathbf{0}$), satisfies the equation

$$\mathbf{A}\mathbf{c} = \lambda\mathbf{c}, \tag{A.10}$$

then λ is said to be an "eigenvalue" of $\mathbf{A}$ and $\mathbf{c}$ is said to be an "eigenvector" corresponding to λ. Equation (A.10) has a non-trivial solution if and only if

$$\det(\mathbf{A} - \lambda\mathbf{1}) = 0, \tag{A.11}$$

which is often referred to in the mathematical physics literature as a "secular equation". The left-hand side of Equation (A.11) is a polynomial $P(\lambda)$ of degree m, known as the "characteristic polynomial", whose coefficients are determined by explicit evaluation of the determinant. The eigenvalues are given therefore by the "characteristic equation"

$$P(\lambda) = 0, \tag{A.12}$$

that is, they are the roots of $P(\lambda)$. Suppose that $P(\lambda)$ has R distinct roots $\lambda_1, \lambda_2, \ldots, \lambda_R$, and that λ_j has multiplicity r_j, $j = 1, 2, \ldots, R$, so that

$$P(\lambda) = (\lambda - \lambda_1)^{r_1}(\lambda - \lambda_2)^{r_2} \ldots (\lambda - \lambda_R)^{r_R}. \tag{A.13}$$

Then the Cayley-Hamilton Theorem states that the matrix $\mathbf{A}$ also satisfies the characteristic equation (Equation (A.12)), that is,

$$P(\mathbf{A}) = (\mathbf{A} - \lambda_1)^{r_1}(\mathbf{A} - \lambda_2)^{r_2} \ldots (\mathbf{A} - \lambda_R)^{r_R} = \mathbf{0}. \tag{A.14}$$

If $\mathbf{A}'$ is related to $\mathbf{A}$ by a similarity transformation $\mathbf{A}' = \mathbf{S}^{-1}\mathbf{A}\mathbf{S}$, where $\mathbf{S}$ is any non-singular $m \times m$ matrix, then Equation (A.10) can be written as

$$\mathbf{A}'(\mathbf{S}^{-1}\mathbf{c}) = \lambda(\mathbf{S}^{-1}\mathbf{c}). \tag{A.15}$$

Thus $\mathbf{A}$ and $\mathbf{A}'$ have the same set of eigenvalues, with identical multiplicities, and, if $\mathbf{c}$ is an eigenvector of $\mathbf{A}$ corresponding to λ then $\mathbf{c}' = \mathbf{S}^{-1}\mathbf{c}$ is an eigenvector of $\mathbf{A}'$ corresponding to λ and vice versa.

The question now arises as to whether $\mathbf{A}'$ can be made diagonal by an appropriate choice of $\mathbf{S}$. If this is so then $\mathbf{A}$ is said to be "diagonalizable". This is certainly true if $\mathbf{A}$ is Hermitian or unitary, and in both of these cases $\mathbf{S}$ can be chosen to be unitary (Gantmacher 1959). As the operators corresponding to physical observables in quantum mechanics are self-adjoint,

whenever the corresponding operator eigenvalue equation is cast in matrix form (as in Appendix B, Section 4) the matrix involved is Hermitian. Thus all the matrices occurring in such a context are automatically diagonalizable. However, non-diagonalizable matrices do occur in various contexts, so it is worthwhile analysing the question of diagonalizability in more detail. The most important result is embodied in the following theorem.

Theorem I An $m \times m$ matrix $\mathbf{A}$ is diagonalizable if and only if $\mathbf{A}$ possesses m linearly independent eigenvectors.

Proof Suppose first that $\mathbf{A}$ is diagonalizable and that $\mathbf{A}' = \mathbf{S}^{-1}\mathbf{A}\mathbf{S}$ is the diagonal form. Then each diagonal element of $\mathbf{A}'$ is an eigenvalue of $\mathbf{A}'$ (and of $\mathbf{A}$) and the eigenvector of $\mathbf{A}'$ corresponding to the eigenvalue A'_{jj} can be taken to be $\mathbf{c}'_j$, where

$$(\mathbf{c}'_j)_{k1} = \begin{cases} 1, & \text{if } j = k, \\ 0, & \text{if } j \neq k. \end{cases} \tag{A.16}$$

Thus $\mathbf{A}'$ possesses m linearly independent eigenvectors $\mathbf{c}'_j$, $j = 1, 2, \ldots, m$, and hence $\mathbf{A}$ possesses m linearly independent eigenvectors $\mathbf{S}\mathbf{c}'_j$, $j = 1, 2, \ldots, m$.

Conversely, suppose that $\mathbf{A}$ possesses m linearly independent eigenvectors $\mathbf{c}_j$, $j = 1, 2, \ldots, m$. Define the $m \times m$ matrix $\mathbf{S}$ by

$$\mathbf{S} = [\, \mathbf{c}_1 \,|\, \mathbf{c}_2 \,|\, \ldots \,|\, \mathbf{c}_m \,],$$

so that $\det \mathbf{S} \neq 0$. By virtue of Equation (A.7), if $\mathbf{c}_j$ is defined by Equations (A.16) then $\mathbf{S}\mathbf{c}'_j = \mathbf{c}_j$, so $\mathbf{c}'_j = \mathbf{S}^{-1}\mathbf{c}_j$ for $j = 1, 2, \ldots, m$. But the set $\mathbf{c}'_j$ $(j = 1, 2, \ldots, m)$ can be eigenvectors of $\mathbf{A}'$ (as required by Equation (A.15)) only if $\mathbf{A}'$ is diagonal, so $\mathbf{A}$ must be diagonalizable.

This theorem implies that if $\mathbf{A}$ is diagonalizable there are r_j linearly independent eigenvectors corresponding to each eigenvalue of multiplicity r_j, whereas if $\mathbf{A}$ is non-diagonalizable at least one eigenvalue has less linearly independent eigenvectors than its multiplicity.

The following examples illustrate the two possible situations. Suppose first that

$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \tag{A.17}$$

which is Hermitian and hence diagonalizable. The characteristic polynomial is $P(\lambda) = (\lambda - 1)^2(\lambda + 1)$. For the eigenvalue $\lambda = 1$, the $(1,1)$ and $(2,1)$ components of Equation (A.10) both give $c_{21} = c_{11}$, while the $(3,1)$ component is trivially satisfied. Thus

$$\begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

are two linearly independent eigenvectors corresponding to eigenvalue $\lambda = 1$. Similarly, for the eigenvalue $\lambda = -1$, the $(1,1)$ and $(2,1)$ components of

Equation (A.10) give $c_{21} = -c_{11}$, while the $(3,1)$ component gives $c_{31} = 0$. Thus

$$\begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}$$

is the *only* linearly independent eigenvalue corresponding to eigenvalue $\lambda = -1$.

As an example of a non-diagonalizable matrix, consider

$$\mathbf{A} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \tag{A.18}$$

for which $P(\lambda) = \lambda^2$. For the eigenvalue $\lambda = 0$, the $(1,1)$ component of Equation (A.10) gives $c_{21} = 0$, while the $(2,1)$ component is trivially satisfied. Thus although $\lambda = 0$ is an eigenvalue of multiplicity 2,

$$\begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

is the *only* linearly independent eigenvector.

There exists a useful criterion for diagonalizability involving the "minimal polynomial" $M(\mathbf{A})$ of $\mathbf{A}$, which is defined as the polynomial of *lowest* degree in $\mathbf{A}$ such that $M(\mathbf{A}) = \mathbf{0}$. In some cases the minimal polynomial is identical to the characteristic polynomial, but otherwise its degree is less than m. It can be shown (Gantmacher 1959) that $M(\mathbf{A})$ is unique and has the form

$$M(\mathbf{A}) = (\mathbf{A} - \lambda_1)^{s_1}(\mathbf{A} - \lambda_2)^{s_2} \ldots (\mathbf{A} - \lambda_R)^{s_R},$$

where $1 \leq s_j \leq r_j$, $j = 1, 2, \ldots, R$, and where λ_j and r_j are as defined in Equation (A.13). (In particular this implies that *every* distinct eigenvalue of $\mathbf{A}$ appears in a factor of $M(\mathbf{A})$.) Moreover, $\mathbf{A}$ is diagonalizable if and only if $s_j = 1$ for *every* $j = 1, 2, \ldots, R$, that is, if and only if $M(\mathbf{A})$ consists only of *linear* factors. This has the corollary that $\mathbf{A}$ is necessarily diagonalizable if every eigenvalue of $\mathbf{A}$ has multiplicity 1.

The examples that were considered above demonstrate this criterion very neatly. For the matrix $\mathbf{A}$ of Equation (A.17),

$$M(\mathbf{A}) = \mathbf{A}^2 - \mathbf{1} = (\mathbf{A} - \mathbf{1})(\mathbf{A} + \mathbf{1}),$$

which has only linear factors, so that $\mathbf{A}$ must be diagonalizable. By contrast, for the matrix $\mathbf{A}$ of Equation (A.18), $M(\mathbf{A}) = \mathbf{A}^2$, so this $\mathbf{A}$ is non-diagonalizable.

Even when $\mathbf{A}$ is not diagonalizable, it can be transformed by an appropriate similarity transformation into a standard form, the "Jordan canonical form". More precisely, for any $m \times m$ matrix $\mathbf{A}$ there exists an $m \times m$ matrix $\mathbf{S}$ such that all the elements of $\mathbf{A}' = \mathbf{S}^{-1}\mathbf{A}\mathbf{S}$ are zero except possibly the A'_{rr}

elements (for $r = 1, 2, \ldots, m$) and the $A'_{r,r+1}$ elements (for $r = 1, 2, \ldots, m-1$). Moreover, $A'_{r,r+1} = 0$ or 1 for all $r = 1, 2, \ldots, m-1$, and

$$A'_{r,r+1} = \begin{cases} 0 \text{ or } 1, & \text{if } A'_{rr} = A'_{r+1,r+1}, \\ 0, & \text{if } A'_{rr} \neq A'_{r+1,r+1}. \end{cases}$$

For example,

$$\mathbf{A}' = \begin{bmatrix} 2 & 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 5 & 1 & 0 \\ 0 & 0 & 0 & 5 & 1 \\ 0 & 0 & 0 & 0 & 5 \end{bmatrix}$$

is in Jordan canonical form. So too is the matrix $\mathbf{A}$ of Equation (A.18). Obviously the eigenvalues of $\mathbf{A}'$ are just the set of diagonal elements A'_{rr}, $r = 1, 2, \ldots, m$. (Clearly the case in which $\mathbf{A}'$ is diagonal is merely a special case in which $A'_{r,r+1} = 0$ for all $r = 1, 2, \ldots, m-1$.)

Appendix B

Vector Spaces

This appendix is intended both to provide an introduction to vector spaces and to give the various notations and conventions that are used throughout this book.

1 The concept of a vector space

A general vector space is obtained by selectively abstracting certain properties of vectors of the three-dimensional Euclidean space $\mathbb{R}^3$.

A vector ψ of $\mathbb{R}^3$ may be specified by a triple of real numbers x_1, x_2 and x_3, that is, $\psi = (x_1, x_2, x_3)$. (In elementary treatments of $\mathbb{R}^3$ it is conventional to indicate a vector by using bold type, but for treatments of higher-dimensional spaces this convention is discontinued. To help avoid confusion, as far as possible vectors in this appendix will be denoted by the Greek letters $\psi, \phi, \chi, \ldots$ and scalars (that is, real or complex numbers) by $a, b, c, \ldots$.) The product of a vector ψ of $\mathbb{R}^3$ with a real number a is defined to be another vector $a\psi$ such that

$$a\psi = (ax_1, ax_2, ax_3), \tag{B.1}$$

from which it follows that if b is any other real number

$$b(a\psi) = (ba)\psi. \tag{B.2}$$

The sum of two vectors $\psi = (x_1, x_2, x_3)$ and $\phi = (y_1, y_2, y_3)$ of $\mathbb{R}^3$ is defined by

$$\psi + \phi = (x_1 + y_1, x_2 + y_2, x_3 + y_3), \tag{B.3}$$

so that

$$\psi + \phi = \phi + \psi. \tag{B.4}$$

Similarly, if $\chi = (z_1, z_2, z_3)$ is any other vector of $\mathbb{R}^3$,

$$\psi + (\phi + \chi) = (\psi + \phi) + \chi. \tag{B.5}$$

With these definitions it is easily verified that

$$a(\psi + \phi) = a\psi + a\phi \tag{B.6}$$

for any real number a and any two vectors ψ and ϕ. Similarly,

$$(a + b)\psi = a\psi + b\psi \tag{B.7}$$

for any real numbers a and b and any ψ. Finally, there exists a vector $0 = (0, 0, 0)$ such that

$$\psi + 0 = \psi \tag{B.8}$$

for every ψ of $\mathbb{R}^3$.

In a *general* vector space V it is assumed that multiplication of vectors by scalar and vector addition can always be defined (though not necessarily by Equations (B.1) and (B.3)) in such a way that the properties in Equations (B.2), (B.4), (B.5), (B.6), (B.7) and (B.8) are retained. The precise definition is as follows:

Definition *Vector space*
A "vector space" V is a collection of elements $\psi, \phi, \chi, \ldots$ (called vectors) for which "scalar multiplication" $a\psi$ is defined for any "scalar" a from a certain set and for any vector ψ, and for which "vector addition" $\psi + \phi$ is defined for all vectors ψ and ϕ, such that

$$\left.\begin{aligned} a(b\psi) &= (ab)\psi, \\ \psi + \phi &= \phi + \psi, \\ \psi + (\phi + \chi) &= (\psi + \phi) + \chi, \\ a(\psi + \phi) &= a\psi + a\phi, \\ (a + b)\psi &= a\psi + b\psi. \end{aligned}\right\}$$

Moreover, there must exist in V a "zero vector" 0 such that

$$\psi + 0 = \psi$$

for all $\psi \in V$. If the set of scalars consists of all real numbers then V is said to be a "real vector space". Similarly, if the set of scalars consists of all complex numbers, V is called a "complex vector space". The set of scalars is often referred to as the "field".

A set of vectors $\psi_1, \psi_2, \ldots, \psi_d$ of V is described as being *linearly dependent* if there exists a set of non-zero scalars (of the appropriate set) $a_1, a_2, \ldots, a_d$ such that

$$a_1\psi_1 + a_2\psi_2 + \ldots + a_d\psi_d = 0. \tag{B.9}$$

Thus the set $\psi_1, \psi_2, \ldots, \psi_d$ is *linearly independent* if the only solution of Equation (B.9) (in the appropriate set of scalars) is $a_1 = a_2 = \ldots = a_d = 0$. If V contains a set of d linearly independent vectors, but every set of $(d+1)$ vectors is linearly dependent, then V is known as a "d-dimensional space". (For example, the vectors of $\mathbb{R}^3$ form a three-dimensional real vector space.) If there

is no limit on the number of linearly independent vectors then V is said to be an "infinite-dimensional space". Finite-dimensional spaces are much easier to deal with and fortunately most of the vector spaces encountered in this book will be of this type.

Let V be a vector space of finite dimension d and let $\psi_1, \psi_2, \ldots, \psi_d$ be any set of linearly independent vectors of V. Then *any* $\psi \in V$ can be uniquely expressed in terms of $\psi_1, \psi_2, \ldots, \psi_d$ by

$$\psi = a_1\psi_1 + a_2\psi_2 + \ldots + a_d\psi_d, \tag{B.10}$$

where $a_1, a_2, \ldots, a_d$ are a set of scalars that depend on ψ. (This follows from the definition just given, for $\psi, \psi_1, \psi_2, \ldots, \psi_d$ must be linearly dependent, so there exists a set of scalars $b, b_1, b_2, \ldots, b_d$ such that $b\psi + b_1\psi_1 + b_2\psi_2 + \ldots + b_d\psi_d = 0$, and not all members of the set $b, b_1, b_2, \ldots, b_d$ are zero. As b must be non-zero, dividing by b and putting $a_j = -b_j/b$ gives Equation (B.10) immediately. The decomposition (Equation (B.10)) is *unique* because if $\psi = \sum_{j=1}^{d} a_j\psi_j$ and $\psi = \sum_{j=1}^{d} a'_j\psi_j$ then $\sum_{j=1}^{d}(a_j - a'_j)\psi_j = 0$, for which the only solution is $a_j = a'_j$ for $j = 1, 2, \ldots, d$, as the vectors $\psi_1, \psi_2, \ldots, \psi_d$ are assumed to be linearly independent.) The set $\psi_1, \psi_2, \ldots, \psi_d$ is therefore said to provide a "basis" for V. In $\mathbb{R}^3$ a very convenient basis is provided by $\psi_1 = (1,0,0), \psi_2 = (0,1,0)$ and $\psi_3 = (0,0,1)$ for, if $\psi = (x_1, x_2, x_3)$, then $\psi = x_1\psi_1 + x_2\psi_2 + x_3\psi_3$.

The set of d vectors $\psi'_1, \psi'_2, \ldots, \psi'_d$ defined in terms of the basis ψ_1, ψ_2, ..., ψ_d by

$$\psi'_n = \sum_{m=1}^{d} S_{mn}\psi_m$$

for $n = 1, 2, \ldots, d$ form a linearly independent set if and only if $\mathbf{S}$ is non-singular. Thus when $\mathbf{S}$ is non-singular $\psi'_1, \psi'_2, \ldots, \psi'_d$ provides an alternative basis for V.

It is occasionally convenient to regard a d-dimensional complex vector space as a $2d$-dimensional real vector space. If $\psi_1, \psi_2, \ldots, \psi_d$ is a basis for the complex space, then $\psi_1, \psi_2, \ldots, \psi_d$, together with $i\psi_1, i\psi_2, \ldots, i\psi_d$, form a basis for the real space. (It should be noted that ψ_j and $i\psi_j$ are linearly independent elements of the real space (although they are linearly dependent in the complex space) as $a\psi_j + bi\psi_j = 0$ has no solution for *real* numbers a and b, other than $a = b = 0$.)

The following examples show some of the widely differing forms of vector space that are encompassed by the definition.

Example I *The three-dimensional complex vector space* $\mathbb{C}^3$

$\mathbb{C}^3$ consists of the set of triples $\psi = (x_1, x_2, x_3)$, where x_1, x_2 and x_3 are *complex* numbers. Scalar multiplication by an arbitrary complex number a is defined by $a\psi = (ax_1, ax_2, ax_3)$ and vector addition is defined by Equation (B.4). The set of vectors $(1,0,0)$, $(0,1,0)$ and $(0,0,1)$ again provides a convenient basis.

Example II *The set of all $N \times N$ traceless anti-Hermitian matrices* ($N > 1$)
Let $\mathbf{A}$ and $\mathbf{B}$ be any two $N \times N$ traceless anti-Hermitian matrices (see Table A.1). Then the scalar product $a\mathbf{A}$ and vector sum $\mathbf{A} + \mathbf{B}$ may be taken to be the scalar product and matrix sum defined in Appendix A, Section 1. Then $a\mathbf{A}$ and $\mathbf{A} + \mathbf{B}$ are $N \times N$ traceless anti-Hermitian matrices, provided that a is real. Thus the set of such matrices form a real vector space, the $N \times N$ matrix $\mathbf{0}$ (all of whose elements are zero) providing the zero element. It should be noted that even though this vector space is real the elements of matrices involved may be complex! As will be seen in Example II of Chapter 8, Section 5, this vector space has an additional structure and forms the Lie algebra su(N) of the linear Lie group SU(N). It is shown there that the dimension of this space is $(N^2 - 1)$.

Example III *Set of all functions defined in* $\mathbb{R}^3$
Let $\psi(\mathbf{r})$ and $\phi(\mathbf{r})$ be any two complex-valued functions defined for all $\mathbf{r} \in \mathbb{R}^3$. Then $\psi + \phi$ is defined in the natural way by $(\psi + \phi)(\mathbf{r}) = \psi(\mathbf{r}) + \phi(\mathbf{r})$ for all $\mathbf{r} \in \mathbb{R}^3$ and, for any complex number a, $a\psi$ is defined by $(a\psi)(\mathbf{r}) = a(\psi(\mathbf{r}))$ for all $\mathbf{r} \in \mathbb{R}^3$. The set of all such functions then forms an infinite-dimensional complex vector space, the zero vector being defined to be the function that is zero for all $\mathbf{r} \in \mathbb{R}^3$.

A "subspace" of a vector space V is a subset of V that is itself a vector space. The subspace is said to be "proper" if its dimension is less than that of V. V is said to be the "direct sum" of two subspaces V_1 and V_2 if every $\phi \in V$ can be written *uniquely* in the form $\phi = \phi_1 + \phi_2$, where $\phi_1 \in V_1$ and $\phi_2 \in V_2$. This implies that V_1 and V_2 have only the zero element of V in common. If $\psi_1, \psi_2, \ldots, \psi_d$ is a basis for V and $1 \leq d' < d$, then $\psi_1, \psi_2, \ldots, \psi_{d'}$ and $\psi_{d'+1}, \ldots, \psi_d$ are bases for two subspaces of V of dimensions d' and $(d - d')$ respectively. Moreover, V is the direct sum of these two subspaces, because if $\phi = \sum_{j=1}^{d} a_j \psi_j$, then $\phi = \phi_1 + \phi_2$, where $\phi_1 = \sum_{j=1}^{d'} a_j \psi_j$ and $\phi_2 = \sum_{j=d'+1}^{d} a_j \psi_j$, this decomposition being unique because the set $a_1, a_2, \ldots, a_d$ depends uniquely on ϕ. The concept of a direct sum can be generalized to more than two subspaces in the obvious way.

2 Inner product spaces

Many vector spaces have the additional attribute of being endowed with an "inner product". Consider first the example of vectors of $\mathbb{R}^3$, in which the inner product is the familiar scalar product. Thus, if $\psi = (x_1, x_2, x_3)$ and $\phi = (y_1, y_2, y_3)$ are any two vectors of $\mathbb{R}^3$, their inner product (ψ, ϕ) is the real number defined by

$$(\psi, \phi) = x_1 y_1 + x_2 y_2 + x_3 y_3.$$

The "length" of $\psi = (x_1, x_2, x_3)$ is given by $\{(x_1)^2 + (x_2)^2 + (x_3)^2\}^{1/2}$, which is real and non-negative. Indeed it is only zero when $\psi = 0$, the zero vector.

It may be denoted by $\|\psi\|$ and will be called the "norm"" of ψ. Clearly $\|\psi\| = \{(\psi, \psi)\}^{1/2}$.

In $\mathbb{C}^3$ (see Example I of the previous section) it is natural to again require that the norm $\|\psi\|$ be always real and non-negative and also that $\|\psi\| = 0$ only when $\psi = 0$. This is achieved by the definition $\|\psi\| = \{|x_1|^2 + |x_2|^2 + |x_3|^2\}^{1/2}$. The identity $\|\psi\| = \{(\psi, \psi)\}^{1/2}$ can be retained if the inner product of any two vectors $\psi = (x_1, x_2, x_3)$ and $\phi = (y_1, y_2, y_3)$ (where the components are now complex numbers) is defined by

$$(\psi, \phi) = x_1^\star y_1 + x_2^\star y_2 + x_3^\star y_3.$$

With this definition

$$(\psi, \phi) = (\phi, \psi)^\star,$$

and for any two complex numbers a and b

$$(a\psi, b\phi) = a^\star b(\psi, \phi).$$

Also, if $\chi = (z_1, z_2, z_3)$, then

$$(\psi + \phi, \chi) = (\psi, \chi) + (\phi, \chi).$$

A general "inner product space" is a vector space possessing an inner product that has the properties exhibited by these examples (even though the definition of this inner product may be quite different). The precise requirements are as follows.

Definition *Inner product space*
A complex vector space V is said to be an "inner product" space if to every pair of vectors ψ and ϕ of V there corresponds a complex number (ψ, ϕ) (called the inner product of ψ with ϕ) such that:

(a) $(\psi, \phi) = (\phi, \psi)^\star$;

(b) $(a\psi, b\phi) = a^\star b(\psi, \phi)$ for any two complex numbers a and b;

(c) $(\psi + \phi, \chi) = (\psi, \chi) + (\phi, \chi)$ for any $\chi \in V$;

(d) $(\psi, \psi) \geq 0$ for all ψ; and

(e) $(\psi, \psi) = 0$ if and only if $\psi = 0$, the zero vector.

If V is a real vector space the inner product is required to be a real number, and in (b) a and b are restricted to being real numbers, but otherwise the requirements (a) to (e) are the same as for a complex space.

An "abstract" inner product space is a space that satisfies all the axioms without possessing a "concrete" realization for the inner product. It should be noted that (a) and (c) imply that

$$(\chi, \psi + \phi) = (\chi, \psi) + (\chi, \phi),$$

so that, by (b),

$$(\chi, a\psi + b\phi) = a(\chi, \psi) + b(\chi, \phi),$$

$$(a\psi + b\phi, \chi) = a^*(\psi, \chi) + b^*(\phi, \chi).$$

Also, (a) implies that (ψ, ψ) is necessarily real (which is implicit in the requirement (d)).

For any inner product space the "norm" $\|\psi\|$ may be defined by

$$\|\psi\| = \{(\psi, \psi)\}^{1/2}.$$

It follows from (b) that

$$\|a\psi\| = |a|\|\psi\|. \tag{B.11}$$

Two other properties that are easily proved (Akhiezer and Glazman 1961) are the "Schwarz inequality" (with strict inequality applying if ϕ and ψ are linearly independent),

$$|(\psi, \phi)| \leq \|\psi\|\|\phi\|,$$

and the "triangle inequality"

$$\|\psi + \phi\| \leq \|\psi\| + \|\phi\|,$$

both valid for any ψ and ϕ of an inner product space.

By analogy with the situation in $\mathbb{R}^3$, the "distance" $d(\psi, \phi)$ between two vectors ψ and ϕ in a general inner product space may be defined by

$$d(\psi, \phi) = \|\psi - \phi\|. \tag{B.12}$$

Then it follows immediately that

(i) $d(\psi, \phi) = d(\phi, \psi)$;

(ii) $d(\psi, \psi) = 0$;

(iii) $d(\psi, \phi) > 0$ if $\psi \neq \phi$; and

(iv) $d(\psi, \phi) \leq d(\psi, \chi) + d(\chi, \phi)$ for any $\psi, \phi, \chi \in V$,

all of which are essential for the interpretation of $d(\psi, \phi)$ as a distance. The distance function $d(\psi, \phi)$ is often called the "metric".

Example I *The d-dimensional complex vector space* $\mathbb{C}^d$

$\mathbb{C}^d$ is the set of d-component quantities $\psi = (x_1, x_2, \ldots, x_d)$, where $x_1, x_2, \ldots, x_d$ are complex numbers. It is a complex vector space of dimension d. The inner product of $\mathbb{C}^d$ may be defined by

$$(\psi, \phi) = \sum_{j=1}^{d} x_j^* y_j, \tag{B.13}$$

where $\psi = (x_1, x_2, \ldots, x_d)$ and $\phi = (y_1, y_2, \ldots, y_d)$, which satisfies all the requirements for $\mathbb{C}^d$ to form an inner product space. From Equations (B.12) and (B.13) it follows that

$$d(\psi, \phi) = \{\textstyle\sum_{j=1}^{d} |x_j - y_j|^2\}^{1/2} .$$

Example II *The set of all $m \times m$ matrices*
The set of all $m \times m$ matrices with complex elements forms a complex vector space of dimension m^2, provided that the scalar product and vector sum are taken to be the scalar product and matrix sum defined in Appendix A, Section 1. The inner product of two such matrices $\mathbf{A}$ and $\mathbf{B}$ may be defined by

$$(\mathbf{A}, \mathbf{B}) = \sum_{j=1}^{m} \sum_{k=1}^{m} A_{jk}^{*} B_{jk}, \tag{B.14}$$

which again satisfies all the requirements for the vector space to form an inner product space. Moreover, Equations (B.12) and (B.14) imply that

$$d(\mathbf{A}, \mathbf{B}) = \{\textstyle\sum_{j=1}^{m} \sum_{k=1}^{m} |A_{jk} - B_{jk}|^2\}^{1/2} .$$

This explains the origin of the metric of Equation (3.1). Comparison of Equations (B.12) and (B.13) shows that this inner product space is essentially just $\mathbb{C}^{m^2}$.

Two elements ψ and ϕ of an inner product space are said to be "orthogonal" if $(\psi, \phi) = 0$. (In $\mathbb{R}^3$ this coincides with the usual geometric notion of orthogonality.) A vector ψ is described as being "normalized" if $\|\psi\| = 1$. An "ortho-normal" set is then a set of vectors $\psi_1, \psi_2, \ldots$ such that $(\psi_j, \psi_k) = \delta_{jk}$ for $j, k = 1, 2, \ldots$. From any set of linearly independent vectors $\phi_1, \phi_2, \ldots$ an ortho-normal set $\psi_1, \psi_2, \ldots$ can be constructed by taking appropriate linear combinations. The procedure, often called the "Schmidt orthogonalization process", is as follows. First let

$$\begin{aligned} \theta_1 &= \phi_1; \\ \theta_2 &= \phi_2 - \{(\theta_1, \phi_2)/(\theta_1, \theta_1)\}\theta_1; \\ \theta_3 &= \phi_3 - \{(\theta_1, \phi_3)/(\theta_1, \theta_1)\}\theta_1 - \{(\theta_2, \phi_3)/(\theta_2, \theta_2)\}\theta_2; \end{aligned}$$

and so on. The vectors $\theta_1, \theta_2, \ldots$ are then mutually orthogonal. Finally let $\psi_j = \{\|\theta_j\|^{-1}\}\theta_j$ for $j = 1, 2, \ldots$, so that, by Equation (B.11), $\|\psi_j\| = \|\theta_j\|^{-1}\|\theta_j\| = 1$. Then $\psi_1, \psi_2, \ldots$ form an ortho-normal set.

Ortho-normal sets are particularly useful as bases. If V is an inner product space of dimension d and the basis $\psi_1, \psi_2, \ldots, \psi_d$ of Equation (B.10) is an ortho-normal set, then forming the inner product of both sides of Equation (B.10) with ψ_j gives

$$(\psi_j, \psi) = \sum_{k=1}^{d} a_k (\psi_j, \psi_k) = \sum_{k=1}^{d} a_k \delta_{jk} = a_j .$$

Thus Equation (B.10) can be rewritten as

$$\psi = \sum_{j=1}^{d} (\psi_j, \psi)\psi_j. \tag{B.15}$$

If $\psi'_1, \psi'_2, \ldots, \psi'_d$ is another basis for V and the $d \times d$ matrix $\mathbf{S}$ is defined by

$$\psi'_n = \sum_{m=1}^{d} S_{mn}\psi_m$$

for $n = 1, 2, \ldots, d$, then $\psi'_1, \psi'_2, \ldots, \psi'_d$ also form an ortho-normal set if and only if $\mathbf{S}$ is a unitary matrix. This follows from the fact that

$$(\psi'_j, \psi'_k) = \sum_{m=1}^{d}\sum_{n=1}^{d} S^{\star}_{mj} S_{nk} (\psi_m, \psi_n) = (\mathbf{S}^{\dagger}\mathbf{S})_{jk}.$$

3 Hilbert spaces

For an infinite-dimensional inner product space it is natural to enquire whether the expansion in Equation (B.15) is valid with the finite sum replaced by an infinite sum. This immediately poses questions of convergence for such infinite series. With the metric introduced in Section 2 one may say that the infinite *sequence* $\phi_1, \phi_2, \ldots$ of vectors in an inner product space V tends to a limit ϕ of V (i.e. $\phi_n \to \phi$ as $n \to \infty$) if and only if $d(\phi_n, \phi) \to 0$ as $n \to \infty$. Then for an infinite *series* one may say that $\sum_{j=1}^{\infty} \psi_j$ converges to ϕ if the sequence of partial sums defined for $n = 1, 2, \ldots$ by $\phi_n = \sum_{j=1}^{n} \psi_j$ converges to ϕ, so that all such questions are reduced to questions about sequences.

A sequence $\phi_1, \phi_2, \ldots$ for which

$$\lim_{m,n\to\infty} d(\phi_n, \phi_m) = 0$$

(where m and n tend to infinity independently) is called a "Cauchy sequence". It follows immediately from property (iv) of the metric $d(\psi, \phi)$ that, if $\phi_1, \phi_2, \ldots$ tends to some limit ϕ, then $\phi_1, \phi_2, \ldots$ must be a Cauchy sequence. Unfortunately, examples can be constructed which demonstrate that, in general, the converse is not true. This makes the general investigation of convergence very difficult, for while it is easy to test whether a sequence is a Cauchy sequence or not, direct examination of the definition of convergence requires some presupposition about the possible limit ϕ. This problem can be completely avoided by confining attention to those spaces for which *every* Cauchy sequence converges, that is, to "Hilbert spaces". The definition will be given for complex inner product spaces, as the only infinite-dimensional spaces that will be met in this book are of this type.

Definition *Hilbert space*
A "Hilbert space" is a complex inner product space in which *every* Cauchy sequence converges to an element of the space.

The following further restriction is required in order that Equation (B.15) may be generalized to the desired form.

Definition *Separable Hilbert space*
A Hilbert space V is said to be "separable" if there exists a *countable* set of elements $\mathcal{S}$ contained in V such that every vector $\psi \in V$ has some element $\phi \in \mathcal{S}$ arbitrarily close to it. That is, for any $\psi \in V$ and any $\epsilon > 0$ there must exist a $\phi \in \mathcal{S}$ such that $d(\phi, \psi) < \epsilon$. The set $\mathcal{S}$ is then said to be "dense" in V.

It is easily shown that every finite-dimensional complex inner product space is a separable Hilbert space.

Definition *Complete ortho-normal system*
An ortho-normal set of vectors $\psi_1, \psi_2, \ldots$ of a Hilbert space is said to be "complete" if there is no non-zero vector that is orthogonal to every ψ_j, $j = 1, 2, \ldots$.

Obviously in an infinite-dimensional Hilbert space a complete set of vectors necessarily contains an infinite number of elements. The following two theorems then provide the required extension of Equation (B.15).

Theorem I If an infinite-dimensional Hilbert space is *separable*, then the space contains a complete ortho-normal system, and every complete ortho-normal system in the space consists of a *countable* number of vectors.

Theorem II If the vectors $\psi_1, \psi_2, \ldots$ form a complete ortho-normal system of an infinite-dimensional Hilbert space, then any vector ψ of the space can be written as

$$\psi = \sum_{j=1}^{\infty} (\psi_j, \psi)\psi_j. \tag{B.16}$$

Moreover,

$$\|\psi\|^2 = \sum_{j=1}^{\infty} |(\psi_j, \psi)|^2, \tag{B.17}$$

Equation (B.17) is often called "Parseval's Relation". Proofs of both theorems may be found in the book of Akhiezer and Glazman (1961).

Example I *The separable Hilbert space* L^2
L^2 is defined to be the set of all complex-valued functions $\phi(\mathbf{r})$ (defined for

all $\mathbf{r} \in \mathbb{R}^3$) such that

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |\phi(\mathbf{r})|^2 \, dx \, dy \, dz$$

exists and is finite, the integral here being the Lebesgue integral (see below). The inner product of L^2 may be defined by

$$(\phi, \psi) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \phi(\mathbf{r})^\star \psi(\mathbf{r}) \, dx \, dy \, dz, \tag{B.18}$$

where the integral is again the Lebesgue integral. With addition and scalar multiplication defined as in Example III of Section 1, it can be shown that L^2 is an infinite-dimensional separable Hilbert space (cf. Akhiezer and Glazman 1961). Equation (B.18) implies that

$$\|\phi\|^2 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |\phi(\mathbf{r})|^2 \, dx \, dy \, dz.$$

For a proper development of the concept of the Lebesgue integral, the reader is referred to specialized texts such as that of Riesz and Sz.-Nagy (1956). However, for the understanding of the present book no detailed knowledge is required. It is sufficient to be aware that the definition of the Lebesgue integral is more general than that of the more familiar Riemann integral, so that functions that are not Riemann-integrable may still be Lebesgue-integrable. Nevertheless, the generalization is such that every Riemann-integrable function is Lebesgue-integrable and the values of the two integrals coincide. Also, if $f(\mathbf{r}) = 0$ except on a "set of measure zero" then

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(\mathbf{r}) \, dx \, dy \, dz = 0.$$

(It is difficult to give a concise characterization of sets of measure zero, but two important facts are easily stated. Firstly, the set of points $\mathbf{r}$ in any sphere $|\mathbf{r} - \mathbf{r}_0|^2 < \delta$ of $\mathbb{R}^3$ has non-zero measure provided $\delta > 0$. Secondly, a set consisting of a finite or a countable number of points has measure zero.) Two functions $f(\mathbf{r})$ and $g(\mathbf{r})$ that are equal except on a set of measure zero are said to be equal "almost everywhere". For such functions

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(\mathbf{r}) \, dx \, dy \, dz = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} g(\mathbf{r}) \, dx \, dy \, dz.$$

Consequently two functions $\psi(\mathbf{r})$ and $\phi(\mathbf{r})$ that are equal almost everywhere are to be regarded as being *identical* members of L^2.

4 Linear operators

Let D be a subset of a separable Hilbert space V. If for every $\psi \in D$ there exists a unique element $\phi \in V$, one can write $\phi = A\psi$, thereby defining the

"operator" A. D is called the "domain" of A, and the set Δ consisting of all $\phi = A\psi$, where ψ runs through all of D, is known as the "range" of A. Two operators A and B are then said to be "equal" if they have the same domain D, and if $A\psi = B\psi$ for all $\psi \in D$.

If the mapping $\phi = A\psi$ is one-to-one, the inverse operator A^{-1} may be defined by $A^{-1}\phi = \psi$ if and only if $\phi = A\psi$. Clearly the domain and range of A^{-1} are Δ and D respectively.

Definition *Linear operator*
An operator A is said to be "linear" if its domain D is a linear manifold (a set D such that if $\phi, \psi \in D$ then $(a\phi + b\psi) \in D$ for all complex numbers a and b) and if

$$A(a\phi + b\psi) = aA\phi + bA\psi$$

for all $\phi, \psi \in D$ and any two complex numbers a and b.

There is no requirement in general that D be the whole Hilbert space, so the definition accommodates such operators as $\partial/\partial x$ acting in $V = L^2$, for which D is the set of functions of L^2 that are differentiable with respect to x.

Definition *Bounded linear operator*
A linear operator A is said to be "bounded" if there exists a positive constant K such that $\|A\psi\| \leq K\|\psi\|$ for all $\psi \in D$.

Theorem I If A is a linear operator acting in a finite-dimensional inner product space V and $D = V$, then A is necessarily bounded.

Definition *Unitary operator*
An operator U is said to be "unitary" if $D = \Delta = V$ and

$$(U\phi, U\psi) = (\phi, \psi)$$

for all $\phi, \psi \in V$.

It is easily shown that every unitary operator is a bounded linear operator. It is obvious that if $\psi_1, \psi_2, \ldots$ form a complete ortho-normal set then $\psi'_j = U\psi_j$, $j = 1, 2, \ldots$ also form a complete ortho-normal set. Conversely, if $\psi_1, \psi_2, \ldots$ and $\psi'_1, \psi'_2, \ldots$ are two complete ortho-normal sets in a Hilbert space V, then there exists a unitary operator U such that $\psi'_j = U\psi_j$, $j = 1, 2, \ldots$.

For a general treatment of linear operators the reader is referred to the books of Akhiezer and Glazman (1961), Simmons (1963) and Riesz and Sz. Nagy (1956). However, as all the operators associated with finite-dimensional representations of groups and Lie algebras are either unitary or act on finite-dimensional spaces, attention here will henceforth be concentrated exclusively on *bounded* linear operators whose domain is the *whole* Hilbert space V.

If A is such an operator there exists an "adjoint" operator $A^\dagger$ whose domain is also V such that

$$(A^\dagger\phi, \psi) = (\phi, A\psi)$$

for all $\phi, \psi \in V$. It is easily shown that $(AB)^\dagger = B^\dagger A^\dagger$, $(A^\dagger)^\dagger = A$, and $U^\dagger = U^{-1}$ for a unitary operator U.

Definition *Self-adjoint operator*
A bounded linear operator A whose domain is the whole Hilbert space V is said to be "self-adjoint" if $A = A^\dagger$, that is, if

$$(A\phi, \psi) = (\phi, A\psi) \tag{B.19}$$

for all $\phi, \psi \in V$.

If for a bounded linear operator A there exists a non-zero vector ψ and a complex number λ such that

$$A\psi = \lambda\psi, \tag{B.20}$$

then ψ is said to be an "eigenvector" of A and λ is referred to as the corresponding "eigenvalue". If there exist d linearly independent eigenvectors $\psi_1, \psi_2, \ldots, \psi_d$ of A with the same eigenvalue λ, then λ is said to have "multiplicity d" or to be "d-fold degenerate". In that case any linear combination $(b_1\psi_1 + b_2\psi_2 + \ldots + b_d\psi_d)$ is also an eigenvector with the same eigenvalue λ.

For the special case of self-adjoint operators there are three important theorems:

Theorem II The eigenvalues of a *self-adjoint* operator are all *real.*

Proof Suppose that $A\psi = \lambda\psi$, where $\psi \neq 0$. Then, if A is self-adjoint, $\lambda(\psi, \psi) = (\psi, A\psi) = (A\psi, \psi) = \lambda^\star(\psi, \psi)$, so $\lambda = \lambda^\star$.

Theorem III Eigenvectors of a *self-adjoint* operator belonging to *different* eigenvalues are *orthogonal.*

Proof Suppose that $A\psi_1 = \lambda_1\psi_1$ and $A\psi_2 = \lambda_2\psi_2$, where $\lambda_1 \neq \lambda_2$. Then, if A is self-adjoint, $\lambda_1(\psi_2, \psi_1) = (\psi_2, A\psi_1) = (A\psi_2, \psi_1) = \lambda_2^\star(\psi_2, \psi_1) = \lambda_2(\psi_2, \psi_1)$, so that $(\lambda_1 - \lambda_2)(\psi_2, \psi_1) = 0$. As $\lambda_1 - \lambda_2 \neq 0$, it follows that $(\psi_2, \psi_1) = 0$.

Theorem IV If A is a self-adjoint operator and U is a unitary operator, then $A' = U^{-1}AU$ is also self-adjoint and possesses exactly the same eigenvalues as A.

Proof A' is self-adjoint because

$$(A')^\dagger = (U^{-1}AU)^\dagger = U^\dagger A^\dagger (U^{-1})^\dagger = U^{-1}AU = A'.$$

Now suppose that ψ' is an eigenvector of A' with eigenvalue λ', so that $A'\psi' = \lambda'\psi'$. Then $U^{-1}AU\psi' = \lambda'\psi'$, so that $A(U\psi') = \lambda'(U\psi')$, showing that $U\psi'$ is an eigenvector of A with the same eigenvalue λ'.

Every bounded operator has a matrix representation. Indeed, the operator eigenvalue equation (Equation (B.20)) can be re-cast in the form of the matrix eigenvalue equation (Equation (A.10)). For convenience, the argument will be presented for a finite-dimensional inner product space V of dimension d, but the results generalize in the obvious way to bounded operators acting on a separable infinite-dimensional Hilbert space, although in that case all the matrices involved are infinite-dimensional.

Let $\psi_1, \psi_2, \ldots, \psi_d$ be an ortho-normal set of V. Taking the inner product of both sides of Equation (B.20) with any ψ_k and invoking Equation (B.15) gives

$$\sum_{j=1}^{d}(\psi_k, A\psi_j)(\psi_j, \psi) = \lambda\sum_{j=1}^{d}(\psi_k, \psi_j)(\psi_j, \psi)\ (= \lambda(\psi_k, \psi)) \tag{B.21}$$

for $k = 1, 2, \ldots, d$. Let $\mathbf{A}$ be the $d \times d$ matrix defined by

$$A_{kj} = (\psi_k, A\psi_j) \tag{B.22}$$

for $j, k = 1, 2, \ldots, d$, and let $\mathbf{c}$ be the $d \times 1$ column matrix whose elements are specified by $c_{j1} = (\psi_j, \psi)$, $j = 1, 2, \ldots, d$. Then Equation (B.21) can be rewritten as $\mathbf{Ac} = \lambda\mathbf{c}$, that is, as Equation (A.10).

It should be noted that if $A\psi_n$ is expanded in terms of the ortho-normal set, then, by Equation (B.15),

$$A\psi_n = \sum_{m=1}^{d}(\psi_m, A\psi_n)\psi_m = \sum_{m=1}^{d} A_{mn}\psi_m. \tag{B.23}$$

It will be observed that the ordering of indices is *exactly* as in Equations (4.1) and (4.4).

If A is a *self-adjoint* operator then its corresponding matrix $\mathbf{A}$ is *Hermitian*, as, by Equations (B.19) and (B.22),

$$A_{kj} = (\psi_k, A\psi_j) = (A\psi_k, \psi_j) = (\psi_j, A\psi_k)^\star = A^\star_{jk}.$$

Similarly, if U is a *unitary* operator and $\mathbf{U}$ is its corresponding matrix, then $\mathbf{U}$ is a *unitary* matrix. (This follows as $(\psi_k, U\psi_j) = (U\psi_j, \psi_k)^\star = (\psi_j, U^{-1}\psi_k)^\star$, so that $U_{kj} = ((\mathbf{U}^{-1})_{jk})^\star$.)

Finally, if A, B and C are three bounded operators such that $C = AB$, and if $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ are their corresponding matrices, then $\mathbf{C} = \mathbf{AB}$. (As $AB\psi_j = C\psi_j$ for each ψ_j, $j = 1, 2, \ldots, d$, then $C_{kj} = (\psi_k, C\psi_j) = (\psi_k, AB\psi_j)$. But, from Equation (B.23), $B\psi_j = \sum_{m=1}^{d}(\psi_m, B\psi_j)\psi_m$, so $C_{kj} = \sum_{m=1}^{d}(\psi_k, A\psi_m)(\psi_m, B\psi_j) = \sum_{m=1}^{d} A_{km}B_{mj}$.) This is the origin of the duality between operators and matrices that is used repeatedly, particularly in Chapter 1, Section 4, and Chapter 4, Section 1.

5 Bilinear forms

Even when a vector space does not possess an inner product it may possess a symmetric non-degenerate bilinear form which gives rise to rather similar properties. In particular this is true of semi-simple Lie algebras (see Chapter 11).

Definition *Symmetric bilinear form*
A *complex* vector space V possesses a symmetric bilinear form B if to every pair of vectors ψ and ϕ of V there corresponds a complex number $B(\psi, \phi)$ such that

(a) $B(\psi, \phi) = B(\phi, \psi)$,

(b) $B(a\psi, b\phi) = abB(\psi, \phi)$, for any two complex numbers a and b,

(c) $B(\psi + \phi, \chi) = B(\psi, \chi) + B(\phi, \chi)$, for any $\chi \in V$.

If V is a *real* vector space the bilinear form $B(\psi, \phi)$ is required to be real for all $\psi, \phi \in V$, and in (b) a and b are restricted to being real numbers, but otherwise the conditions (a) to (c) are the same as for a complex space.

It should be noted that (a), (b) and (c) imply that

$$B(\chi, a\psi + b\phi) = aB(\chi, \psi) + bB(\chi, \phi)$$

and

$$B(a\psi + b\phi, \chi) = aB(\psi, \chi) + bB(\phi, \chi).$$

There is no requirement that $B(\psi, \psi)$ be real (unless V is a real vector space), and even then $B(\psi, \psi)$ could be negative, or could be zero with $\psi \neq 0$.

Thus a symmetric bilinear form does *not* in general have the properties of an inner product (as defined in Section 2). Conversely, if V is a *complex* inner product space then the inner product is not a symmetric bilinear form (because the right-hand sides of parts (a) and (b) of the definition in Section 2 of an inner product involve complex conjugation, whereas the corresponding parts (a) and (b) of the definition of a symmetric bilinear form do not do so). However, if V is a *real* inner product space these particular distinctions disappear, so in this case an inner product is also a symmetric bilinear form.

Let $\psi_1, \psi_2, \ldots, \psi_d$ be a basis for V, and let $\mathbf{B}$ be the $d \times d$ matrix defined by

$$B_{pq} = B(\psi_p, \psi_q), \quad p, q = 1, 2, \ldots, d. \tag{B.24}$$

Then, if $\psi = \sum_{j=1}^{d} a_j \psi_j$ and $\phi = \sum_{k=1}^{d} b_k \psi_k$,

$$B(\psi, \phi) = \sum_{j=1}^{d} \sum_{k=1}^{d} B_{jk} a_j b_k. \tag{B.25}$$

Suppose that $\psi'_1, \psi'_2, \ldots, \psi'_d$ is another basis for V, with

$$\psi'_n = \sum_{m=1}^{d} S_{mn}\psi_m,$$

$(n = 1, 2, \ldots, d)$, so that (as noted in Section 1) $\mathbf{S}$ is a $d \times d$ non-singular matrix. Let $\mathbf{B}'$ be the corresponding matrix for the bilinear form defined for this basis, that is, let

$$B'_{pq} = B(\psi'_p, \psi'_q), \quad p, q = 1, 2, \ldots, d.$$

Then a very straightforward argument shows that

$$\mathbf{B}' = \tilde{\mathbf{S}}\mathbf{B}\mathbf{S}.$$

This implies that $\det \mathbf{B}' = (\det \mathbf{S})^2 \det \mathbf{B}$. Consequently $\det \mathbf{B}' = 0$ if and only if $\det \mathbf{B} = 0$.

If V is a real vector space it can be shown (Gantmacher 1959) that $\mathbf{S}$ may be chosen so that $\mathbf{B}'$ is diagonal with diagonal elements $1, -1$, or 0 only. Then, if the basis $\psi'_1, \psi'_2, \ldots, \psi'_d$ is ordered so that the first $d_+ (\geq 0)$ members correspond to 1, the next $d_- (\geq 0)$ to -1, and the remaining $d_0 (\geq 0)$ to 0, and if $\psi = \sum_{j=1}^{d} a'_j \psi'_j$ and $\phi = \sum_{j=1}^{d} b'_j \psi'_j$, then

$$B(\psi, \phi) = \sum_{j=1}^{d_+} a'_j b'_j - \sum_{j=d_+ +1}^{d_+ + d_-} a'_j b'_j. \tag{B.26}$$

Matrices $\mathbf{S}$ with this property can be chosen in an infinite number of ways, but all choices give the same values of the dimensions d_+, d_- and d_0 (Gantmacher 1959). The invariant quantity $\sigma = d_+ - d_-$ is called the "signature" of the bilinear form.

Definition *Degenerate and non-degenerate symmetric bilinear forms*
A symmetric bilinear form B is said to be "degenerate" if there exists in V some $\psi \neq 0$ such that $B(\psi, \phi) = 0$ for *all* $\phi \in V$. Conversely, a symmetric bilinear form is "non-degenerate" if, for each $\psi \in V$, the condition

$$B(\psi, \phi) = 0 \text{ for all } \phi \in V$$

implies that $\psi = 0$.

Theorem I The symmetric bilinear form B is *non-degenerate* if and only if $\det \mathbf{B} \neq 0$, where $\mathbf{B}$ is the $d \times d$ matrix defined in Equation (B.24).

Proof It should be noted that as $\det \mathbf{B}' = 0$ if and only if $\det \mathbf{B} = 0$, this condition for non-degeneracy is actually independent of the choice of basis, as is to be expected.

Suppose that there exists a $\psi \in V$ such that $B(\psi, \phi) = 0$ for *all* $\phi \in V$. By Equation (B.25) this is so if and only if $\sum_{j,k=1}^{d} B_{jk} a_j b_k = 0$ for all sets $b_1, b_2, \ldots, b_d$, that is, if and only if $\sum_{j=1}^{d} B_{jk} a_j = 0$ for each $k = 1, 2, \ldots, d$. As this set of d simultaneous linear equations for $a_1, a_2, \ldots, a_d$ has a non-trivial solution (i.e. a solution other than $\psi = 0$) if and only if $\det \mathbf{B} = 0$, the quoted result follows.

6 Linear functionals

The theory of linear functionals will be considered here only for finite-dimensional vector spaces and inner product spaces. The results will be needed in the discussions of Lie algebras in Chapter 13. The generalization to infinite-dimensional Hilbert spaces may be found in the books of Akhiezer and Glazman (1961) and Riesz and Sz. Nagy (1956).

Definition *Linear functional*
If to every member ψ of a *complex* finite-dimensional vector space V a *complex number* $\Phi(\psi)$ is assigned in such a way that

$$\Phi(a\phi + b\psi) = a\Phi(\phi) + b\Phi(\psi) \tag{B.27}$$

for every $\phi, \psi \in V$ and any two complex numbers a and b, then Φ is said to be a "linear functional" on V. Likewise, a linear functional on a *real* finite-dimensional vector space V is an assignment of a *real number* $\Phi(\psi)$ to every $\psi \in V$ such that Equation (B.27) holds for every $\phi, \psi \in V$ and any two real numbers a and b.

If Φ and Ψ are any two linear functionals defined on a finite-dimensional vector space V, then $(\Phi + \Psi)$ may be defined by $(\Phi + \Psi)(\psi) = \Phi(\psi) + \Psi(\psi)$ for all $\psi \in V$. Similarly, $a\Phi$ may be defined by $(a\Phi)(\psi) = a(\Phi(\psi))$ for all $\psi \in V$, a being any real or complex number as appropriate. Then the set of linear functionals on V themselves form a vector space $V^\star$, called the "dual" of V. (The zero of $V^\star$ is the functional whose value is 0 for all $\psi \in V$.) $V^\star$ is real when V is real and is complex when V is complex.

Suppose that V has dimension d and $\psi_1, \psi_2, \ldots, \psi_d$ is a basis for V. Then each linear functional Φ on V is completely specified by the d numbers $\Phi(\psi_j)$, $j = 1, 2, \ldots, d$. (*Any* $\psi \in V$ can be written in the form of Equation (B.10) as $\psi = \sum_{j=1}^{d} a_j \psi_j$, so, by Equation (B.27), $\Phi(\psi) = \sum_{j=1}^{d} a_j \Phi(\psi_j)$.) Let Φ_k, $k = 1, 2, \ldots, d$, be a set of linear functionals defined by

$$\Phi_k(\psi_j) = \delta_{jk} \tag{B.28}$$

for all $j, k = 1, 2, \ldots, d$. The functionals of this set are obviously linearly independent. Moreover, if Φ is *any* linear functional on V, then Equation (B.28) implies that $\Phi = \sum_{k=1}^{d} \Phi(\psi_k)\Phi_k$, that is, Φ depends linearly on $\Phi_1, \Phi_2, \ldots, \Phi_d$. Thus the dual space $V^\star$ has the same dimension d as V, and $\Phi_1, \Phi_2, \ldots, \Phi_d$ provide a basis for $V^\star$.

If V is equipped with a symmetric non-degenerate bilinear form, or is an inner product space, the following theorems show that every linear functional is given by a remarkably simple expression.

Theorem I Each linear functional Φ on a finite-dimensional vector space equipped with a symmetric non-degenerate bilinear form can be expressed in the form

$$\Phi(\psi) = B(\psi_\Phi, \psi) \tag{B.29}$$

for all $\psi \in V$, where $B(\psi_\Phi, \psi)$ is the bilinear form, and ψ_Φ is an element of V which is uniquely determined by the functional Φ.

Proof Suppose that $\psi_\Phi = \sum_{j=1}^{d} a_j \psi_j$ has the required property, ψ_1, ψ_2, ..., ψ_d being a basis for V. Then Equation (B.29) can be written in the form $\Phi(\psi) = \sum_{j=1}^{d} B(\psi_j, \psi) a_j$, so that for each $k = 1, 2, \ldots, d$,

$$\Phi(\psi_k) = \sum_{j=1}^{d} B(\psi_j, \psi_k) a_j.$$

Thus if $\mathbf{\Phi}$ and $\mathbf{a}$ are the $d \times 1$ matrices with elements $\Phi(\psi_k)$ and a_k respectively ($k = 1, 2, \ldots, d$), and $\mathbf{B}$ is defined by Equation (B.24), as $\mathbf{B}$ is symmetric these equations can be written as $\mathbf{\Phi} = \mathbf{Ba}$. The linear functional Φ fixes $\mathbf{\Phi}$. This equation has a *unique* solution $\mathbf{a}$ when $\det \mathbf{B} \neq 0$, namely $\mathbf{a} = \mathbf{B}^{-1}\mathbf{\Phi}$, which then determines ψ_Φ uniquely.

Theorem II Each linear functional Φ on a Hilbert space V can be expressed in the form

$$\Phi(\psi) = (\psi_\Phi, \psi)$$

for all $\psi \in V$, where (ψ_Φ, ψ) is the inner product of V, and ψ_Φ is an element of V which is uniquely determined by the functional Φ.

Proof If V is finite-dimensional, a proof can be given along the lines of that of the previous theorem. For the infinite-dimensional case see Akhiezer and Glazman (1961) or Riesz and Sz. Nagy (1956).

This latter theorem is often called the "Riesz Representation Theorem". It is easily verified that if ψ_Φ is as specified in this theorem and $\psi_1, \psi_2, \ldots$ is an ortho-normal basis for V, then

$$\psi_\Phi = \sum_j \Phi(\psi_j)^* \psi_j.$$

7 Direct product spaces

Let V_1 and V_2 be two complex inner product spaces of dimensions d_1 and d_2. Let ψ_j ($j = 1, 2, \ldots, d_1$) and ϕ_s ($s = 1, 2, \ldots, d_2$) be ortho-normal bases for

V_1 and V_2 respectively. Then the "direct product" or "tensor product" space $V_1 \otimes V_2$ may be defined as the complex vector space having the set of $d_1 d_2$ "products" $\psi_j \otimes \phi_s$ as its basis, so that $V_1 \otimes V_2$ is the set of all quantities θ of the form

$$\theta = \sum_{j=1}^{d_1} \sum_{s=1}^{d_2} a_{js} \psi_j \otimes \phi_s, \tag{B.30}$$

where the a_{js} are a set of complex numbers. The direct product of any two elements $\psi = \sum_{j=1}^{d_1} b_j \psi_j$ and $\phi = \sum_{s=1}^{d_2} c_s \phi_s$ of V_1 and V_2 is defined to be

$$\psi \otimes \phi = \sum_{j=1}^{d_1} \sum_{s=1}^{d_2} b_j c_s \psi_j \otimes \phi_s, \tag{B.31}$$

so that the set of such products is a subset of $V_1 \otimes V_2$. It is easily verified that all the requirements for $V_1 \otimes V_2$ to be a vector space are satisfied. (The zero vector of $V_1 \otimes V_2$ corresponds to $a_{js} = 0$ for all $j = 1, 2, \ldots, d_1$, and $s = 1, 2, \ldots, d_2$.) The products $\psi_j \otimes \phi_s$ are assumed to be linearly independent, so that $V_1 \otimes V_2$ has dimension $d_1 d_2$. (This is assumed to be the case even when V_1 and V_2 are identical, when one could take $\psi_j = \phi_j$ for $j = 1, 2, \ldots, d_1 (= d_2)$, implying that the products $\psi_j \otimes \psi_s$ and $\psi_s \otimes \psi_j$ are linearly independent.)

An inner product can be defined on $V_1 \otimes V_2$ by *assuming* that the basis elements $\psi_j \otimes \phi_s$ are ortho-normal, i.e. that

$$(\psi_j \otimes \phi_s, \psi_k \otimes \phi_t) = \delta_{jk} \delta_{st}. \tag{B.32}$$

Then if θ is defined as in Equation (B.30), and

$$\chi = \sum_{j=1}^{d_1} \sum_{s=1}^{d_2} d_{js} \psi_j \otimes \phi_s, \tag{B.33}$$

it follows that

$$(\theta, \chi) = \sum_{j=1}^{d_1} \sum_{s=1}^{d_2} a_{js}^{\star} d_{js}. \tag{B.34}$$

This inner product has all the required properties of an inner product space.

The definition of $V_1 \otimes V_2$ and its inner product of Equation (B.34) is actually *independent* of the choice of the ortho-normal bases of V_1 and V_2. To see this let ψ'_k $(k = 1, 2, \ldots, d_1)$ and ϕ'_t $(t = 1, 2, \ldots, d_2)$ be another pair of ortho-normal bases for V_1 and V_2 respectively. Then (see Section 2) there exists a $d_1 \times d_1$ unitary matrix $\mathbf{F}$ and a $d_2 \times d_2$ unitary matrix $\mathbf{G}$ such that

$$\psi'_j = \sum_{k=1}^{d_1} F_{kj} \psi'_k, \quad j = 1, 2, \ldots, d_1,$$

and

$$\phi'_s = \sum_{t=1}^{d_2} F_{ts} \phi'_t, \quad s = 1, 2, \ldots, d_2.$$

Then, for any θ of $V_1 \otimes V_2$, defined as in Equation (B.30),

$$\theta = \sum_{k=1}^{d_1} \sum_{t=1}^{d_2} a'_{kt} \psi'_k \otimes \phi'_t,$$

where

$$a'_{kt} = \sum_{l=1}^{d_1} \sum_{u=1}^{d_2} F_{kl} a_{lu} G_{tu},$$

hereby demonstrating that the set $\psi'_k \otimes \phi'_t$ forms an alternative basis for $V_1 \otimes V_2$. Moreover, as the vector χ of Equation (B.33) can similarly be rewritten as

$$\chi = \sum_{k=1}^{d_1} \sum_{t=1}^{d_2} d'_{kt} \psi'_k \otimes \phi'_t,$$

with

$$d'_{kt} = \sum_{l=1}^{d_1} \sum_{u=1}^{d_2} F_{kl} d_{lu} G_{tu},$$

and as $\mathbf{F}$ and $\mathbf{G}$ are unitary, it follows that

$$(\theta, \chi) = \sum_{k=1}^{d_1} \sum_{t=1}^{d_2} a'^{\star}_{kt} d'_{kt},$$

showing that the inner product is independent of the choice of basis (see Equation (B.34)).

In the physics literature the $\otimes$ sign is often omitted in products such as $\psi_j \otimes \phi_s$, but it will be retained throughout this book as a warning that the product is *not* ordinary multiplication.

For abstract inner product spaces V_1 and V_2, the product $\otimes$ in $\psi_j \otimes \phi_s$ neither requires nor is amenable to any further specification. However, in concrete examples this product can be defined quite naturally.

As a first example, suppose $V_1 = \mathbb{C}^3$ and $V_2 = \mathbb{C}^2$, with $\psi_1 = (1,0,0)$, $\psi_2 = (0,1,0)$, $\psi_3 = (0,0,1)$ and $\phi_1 = (1,0), \phi_2 = (0,1)$. Then the products $\psi_j \otimes \phi_s$ can be *defined* as the six-component quantities:

$$\left.\begin{array}{llll} \psi_1 \otimes \phi_1 = (1,0,0,0,0,0), & \psi_1 \otimes \phi_2 = (0,0,0,1,0,0), \\ \psi_2 \otimes \phi_1 = (0,1,0,0,0,0), & \psi_2 \otimes \phi_2 = (0,0,0,0,1,0), \\ \psi_3 \otimes \phi_1 = (0,0,1,0,0,0), & \psi_3 \otimes \phi_2 = (0,0,0,0,0,1), \end{array}\right\}$$

so that Equation (B.32) is satisfied. Clearly $\mathbb{C}^3 \otimes \mathbb{C}^2$ can be identified with $\mathbb{C}^6$.

As a second example, let V_1 and V_2 be subspaces of L^2, the elements of V_1 being functions $\psi(\mathbf{r}_1)$ of $\mathbf{r}_1$ and the elements of V_2 being functions $\phi(\mathbf{r}_2)$ of $\mathbf{r}_2$. Then the elements of $V_1 \otimes V_2$ are linear combinations of products $\psi(\mathbf{r}_1)\phi(\mathbf{r}_2)$, the inner product for which may be defined by

$$\begin{aligned} &(\psi'(\mathbf{r}_1)\phi'(\mathbf{r}_2), \psi(\mathbf{r}_1)\phi(\mathbf{r}_2)) \\ &= \int\int\int\int\int\int dx_1\, dy_1\, dz_1\, dx_2\, dy_2\, dz_2\, \psi'^{\star}(\mathbf{r}_1)\phi'^{\star}(\mathbf{r}_2)\psi(\mathbf{r}_1)\phi(\mathbf{r}_2). \end{aligned}$$

As a final example, let V_1 be a subspace of L^2, consisting of functions $\psi(\mathbf{r})$, and let V_2 be the two-dimensional space of 2×1 matrices with constant entries. Let $\psi_j(\mathbf{r})$ $(j = 1, 2, \ldots, d_1)$ be an orthonormal basis of V_1 and let

$$\phi_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \phi_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix},$$

be an ortho-normal basis of V_2 (it being assumed that the inner product of two elements

$$\begin{bmatrix} a \\ b \end{bmatrix}, \text{ and } \begin{bmatrix} a' \\ b' \end{bmatrix}$$

of V_2 is $(a^\star a' + b^\star b')$). Then $V_1 \otimes V_2$ is the set of two-component quantities

$$\begin{bmatrix} \psi(\mathbf{r}) \\ \psi'(\mathbf{r}) \end{bmatrix}$$

$(\psi(\mathbf{r}), \psi'(\mathbf{r}) \in V_1)$ with inner product defined by

$$\left(\begin{bmatrix} \psi(\mathbf{r}) \\ \psi'(\mathbf{r}) \end{bmatrix}, \begin{bmatrix} \eta(\mathbf{r}) \\ \eta'(\mathbf{r}) \end{bmatrix} \right) = \int\int\int \{\psi^\star(\mathbf{r})\eta(\mathbf{r}) + \psi'^\star(\mathbf{r})\eta'(\mathbf{r})\}\, dx\, dy\, dz$$

for all $\psi(\mathbf{r}), \psi'(\mathbf{r}), \eta(\mathbf{r}), \eta'(\mathbf{r}) \in V_1$.

It is shown in Chapter 5, Section 4, that if V_1 and V_2 are both subspaces of L^2 consisting of functions of the *same* variable $\mathbf{r}$, then it may *not* be possible to identify $V_1 \otimes V_2$ with the set of linear combinations of ordinary products of members of V_1 and V_2 and at the same time retain the inner product of L^2 as the inner product of $V_1 \otimes V_2$.

Appendix C

Character Tables for the Crystallographic Point Groups

The 32 crystallographic point groups of three-dimensional Euclidean space $\mathbb{R}^3$ will be listed in roughly decreasing order of complexity. For each group the following details are given:

(a) *The group elements.* The notation for rotations is as in Chapter 1, 2(a), C_{nj} denoting a proper rotation through $2\pi/n$ in the right-hand screw sense about the axis Oj and I denoting the spatial inversion operator. All the axes involved are indicated in Figures C.1 and C.2. The matrices $\mathbf{R}(T)$ for every relevant proper rotation are specified in Table C.1. The rotations are listed in classes.

(b) *The character table.* Several alternative systems of labelling are given, the first column merely giving an arbitrary listing. In the labelling of the second column one-dimensional representations are denoted by A or B, two-dimensional irreducible representations by E and three-dimensional irreducible representations by T, in all cases with subscripts and/or superscripts attached. (The subscripts g and u (standing for *gerade* and *ungerade*) indicate representations that are even and odd under I respectively.) However, each member of a pair of one-dimensional complex conjugate representations is given the same label, as they correspond to degenerate eigenvalues. (See, for example, Chapter 6, Section 5(a), and Chapter 7, Section 3(f), of Cornwell (1984).)

For a point group that is isomorphic to a group $\mathcal{G}_0(\mathbf{k})$ (see Chapter 7, Section 7(a)) for O_h^1, O_h^5, and O_h^9, the third column gives the labelling convention of Bouckaert *et al.* (1936). In such cases the corresponding $\mathbf{k}$-vector is as defined in Tables 7.2, 7.3, and 7.4. As described in Chapter 7, Section 7(b), it is possible for two or more $\mathbf{k}$-vectors in different stars

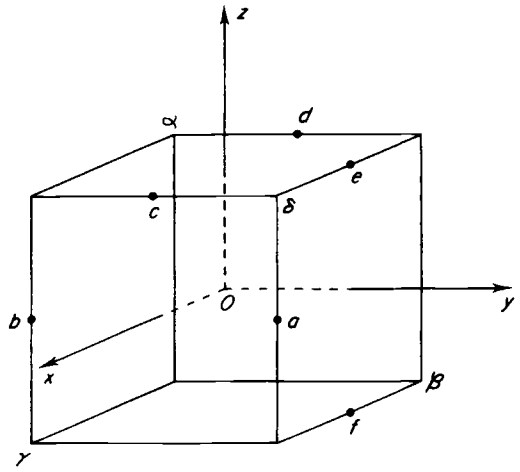

Figure C.1: The axes $Oa, Ob, Oc, Od, Oe, Of, O\alpha, O\beta, O\gamma$ and $O\delta$.

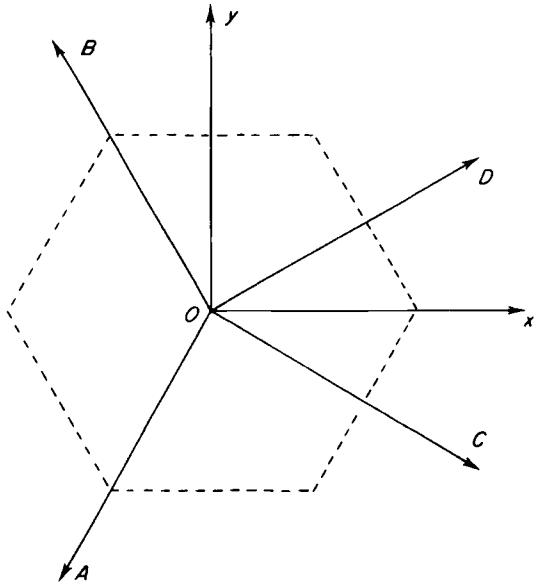

Figure C.2: The axes OA, OB, OC, OD. (All these axes lie in the plane Oxy.)

to have point groups $\mathcal{G}_0(\mathbf{k})$ that are isomorphic. The group elements for each such $\mathcal{G}_0(\mathbf{k})$ belonging to O_h^1, O_h^5, and O_h^9 are specified when this occurs.

(c) *Matrices for the irreducible representations of dimension greater than one.* (Of course these are only unique up to a similarity transformation). For one-dimensional representations the characters themselves are the matrix elements.

The notation employed for the point groups is that of Schönfliess (1923). More information on these groups may be found in the book of Koster *et al.* (1964), which is wholly devoted to this subject, and the articles of Altmann (1962, 1963).

(1) O_h:

(a) Classes [for $\mathcal{G}_0(\mathbf{k})$ of Γ, H, and R]:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{3\alpha}, C_{3\beta}, C_{3\gamma}, C_{3\delta}, C_{3\alpha}^{-1}, C_{3\beta}^{-1}, C_{3\gamma}^{-1}, C_{3\delta}^{-1}$;
$\mathcal{C}_3 = C_{2x}, C_{2y}, C_{2z}$; $\mathcal{C}_4 = C_{4x}, C_{4y}, C_{4z}, C_{4x}^{-1}, C_{4y}^{-1}, C_{4z}^{-1}$;
$\mathcal{C}_5 = C_{2a}, C_{2b}, C_{2c}, C_{2d}, C_{2e}, C_{2f}$; $\mathcal{C}_6 = I$;
$\mathcal{C}_7 = IC_{3\alpha}, IC_{3\beta}, IC_{3\gamma}, IC_{3\delta}, IC_{3\alpha}^{-1}, IC_{3\beta}^{-1}, IC_{3\gamma}^{-1}, IC_{3\delta}^{-1}$;
$\mathcal{C}_8 = IC_{2x}, IC_{2y}, IC_{2z}$; $\mathcal{C}_9 = IC_{4x}, IC_{4y}, IC_{4z}, IC_{4x}^{-1}, IC_{4y}^{-1}, IC_{4z}^{-1}$;
$\mathcal{C}_{10} = IC_{2a}, IC_{2b}, IC_{2c}, IC_{2d}, IC_{2e}, IC_{2f}$.

(b) The character table is given in Table C.2.

(c) Matrices for irreducible representations of dimension greater than one, for any proper rotation C_{nj} of O_h:

$$\begin{array}{lcll}
\mathbf{\Gamma}^3(C_{nj}) & = & \mathbf{\Gamma}^8(C_{nj}) & = \mathbf{\Gamma}''(C_{nj}); \\
\mathbf{\Gamma}^3(IC_{nj}) & = & -\mathbf{\Gamma}^8(IC_{nj}) & = \mathbf{\Gamma}''(C_{nj}); \\
\mathbf{\Gamma}^4(C_{nj}) & = & \mathbf{\Gamma}^9(C_{nj}) & = \mathbf{R}(C_{nj}); \\
\mathbf{\Gamma}^4(IC_{nj}) & = & -\mathbf{\Gamma}^9(IC_{nj}) & = \mathbf{R}(C_{nj}); \\
\mathbf{\Gamma}^5(C_{nj}) & = & \mathbf{\Gamma}^{10}(C_{nj}) & = \mathbf{\Gamma}'(C_{nj}); \\
\mathbf{\Gamma}^5(IC_{nj}) & = & -\mathbf{\Gamma}^{10}(IC_{nj}) & = \mathbf{\Gamma}'(C_{nj});
\end{array}$$

where the matrices $\mathbf{\Gamma}'(C_{nj})$, $\mathbf{\Gamma}''(C_{nj})$ and $\mathbf{R}(C_{nj})$ are given in Tables C.3, C.4, and C.1.

(2) D_{6h}:

(a) Classes [for $\mathcal{G}_0(\mathbf{k})$ of Γ, H, and R]:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{6z}, C_{6z}^{-1}$; $\mathcal{C}_3 = C_{3z}, C_{3z}^{-1}$;
$\mathcal{C}_4 = C_{2z}$; $\mathcal{C}_5 = C_{2x}, C_{2A}, C_{2B}$; $\mathcal{C}_6 = C_{2y}, C_{2C}, C_{2D}$;
$\mathcal{C}_7 = I$; $\mathcal{C}_8 = IC_{6z}, IC_{6z}^{-1}$; $\mathcal{C}_9 = IC_{3z}, IC_{3z}^{-1}$;
$\mathcal{C}_{10} = IC_{2z}$; $\mathcal{C}_{11} = IC_{2x}, IC_{2A}, IC_{2B}$; $\mathcal{C}_{12} = IC_{2y}, IC_{2C}, IC_{2D}$.

(b) The character table is given in Table C.5.

$$\mathbf{R}(E) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad \mathbf{R}(C_{2x}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix},$$

$$\mathbf{R}(C_{2y}) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \qquad \mathbf{R}(C_{2z}) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

$$\mathbf{R}(C_{4x}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}, \qquad \mathbf{R}(C_{4x}^{-1}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix},$$

$$\mathbf{R}(C_{4y}) = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \qquad \mathbf{R}(C_{4y}^{-1}) = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix},$$

$$\mathbf{R}(C_{4z}) = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad \mathbf{R}(C_{4z}^{-1}) = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

$$\mathbf{R}(C_{2a}) = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \qquad \mathbf{R}(C_{2b}) = \begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix},$$

$$\mathbf{R}(C_{2c}) = \begin{bmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \qquad \mathbf{R}(C_{2d}) = \begin{bmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{bmatrix},$$

$$\mathbf{R}(C_{2e}) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \qquad \mathbf{R}(C_{2f}) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix},$$

$$\mathbf{R}(C_{3\alpha}) = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{bmatrix}, \qquad \mathbf{R}(C_{3\beta}) = \begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{bmatrix},$$

$$\mathbf{R}(C_{3\gamma}) = \begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{bmatrix}, \qquad \mathbf{R}(C_{3\delta}) = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix},$$

$$\mathbf{R}(C_{3\alpha}^{-1}) = \begin{bmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{bmatrix}, \qquad \mathbf{R}(C_{3\beta}^{-1}) = \begin{bmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{bmatrix},$$

$$\mathbf{R}(C_{3\gamma}^{-1}) = \begin{bmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \qquad \mathbf{R}(C_{3\delta}^{-1}) = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix},$$

$$\mathbf{R}(C_{3z}) = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} & 0 \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad \mathbf{R}(C_{3z}^{-1}) = \begin{bmatrix} -\frac{1}{2} & -\frac{1}{2}\sqrt{3} & 0 \\ \frac{1}{2}\sqrt{3} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

$$\mathbf{R}(C_{6z}) = \begin{bmatrix} \frac{1}{2} & \frac{1}{2}\sqrt{3} & 0 \\ -\frac{1}{2}\sqrt{3} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad \mathbf{R}(C_{6z}^{-1}) = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2}\sqrt{3} & 0 \\ \frac{1}{2}\sqrt{3} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

$$\mathbf{R}(C_{2A}) = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} & 0 \\ \frac{1}{2}\sqrt{3} & \frac{1}{2} & 0 \\ 0 & 0 & -1 \end{bmatrix}, \qquad \mathbf{R}(C_{2B}) = \begin{bmatrix} -\frac{1}{2} & -\frac{1}{2}\sqrt{3} & 0 \\ -\frac{1}{2}\sqrt{3} & \frac{1}{2} & 0 \\ 0 & 0 & -1 \end{bmatrix},$$

$$\mathbf{R}(C_{2C}) = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2}\sqrt{3} & 0 \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} & 0 \\ 0 & 0 & -1 \end{bmatrix}, \qquad \mathbf{R}(C_{2D}) = \begin{bmatrix} \frac{1}{2} & \frac{1}{2}\sqrt{3} & 0 \\ \frac{1}{2}\sqrt{3} & -\frac{1}{2} & 0 \\ 0 & 0 & -1 \end{bmatrix}.$$

Table C.1: The matrices $\mathbf{R}(T)$ for the proper rotations T appearing in various crystallographic point groups.

			$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$	$\mathcal{C}_4$	$\mathcal{C}_5$	$\mathcal{C}_6$	$\mathcal{C}_7$	$\mathcal{C}_8$	$\mathcal{C}_9$	$\mathcal{C}_{10}$
$\mathbf{\Gamma}^1$	A_{1g}	$\Gamma_1\ H_1\ R_1$	1	1	1	1	1	1	1	1	1	1
$\mathbf{\Gamma}^2$	A_{2g}	$\Gamma_2\ H_2\ R_2$	1	1	1	-1	-1	1	1	1	-1	-1
$\mathbf{\Gamma}^3$	E_g	$\Gamma_{12}\ H_{12}\ R_{12}$	2	-1	2	0	0	2	-1	2	0	0
$\mathbf{\Gamma}^4$	T_{1g}	$\Gamma_{15'}\ H_{15'}\ R_{15'}$	3	0	-1	1	-1	3	0	-1	1	-1
$\mathbf{\Gamma}^5$	T_{2g}	$\Gamma_{25'}\ H_{25'}\ R_{25'}$	3	0	-1	-1	1	3	0	-1	-1	1
$\mathbf{\Gamma}^6$	A_{1u}	$\Gamma_{1'}\ H_{1'}\ R_{1'}$	1	1	1	1	1	-1	-1	-1	-1	-1
$\mathbf{\Gamma}^7$	A_{2u}	$\Gamma_{2'}\ H_{2'}\ R_{2'}$	1	1	1	-1	-1	-1	-1	-1	1	1
$\mathbf{\Gamma}^8$	E_u	$\Gamma_{12'}\ H_{12'}\ R_{12'}$	2	-1	2	0	0	-2	1	-2	0	0
$\mathbf{\Gamma}^9$	T_{1u}	$\Gamma_{15}\ H_{15}\ R_{15}$	3	0	-1	1	-1	-3	0	1	-1	1
$\mathbf{\Gamma}^{10}$	T_{2u}	$\Gamma_{25}\ H_{25}\ R_{25}$	3	0	-1	-1	1	-3	0	1	1	-1

Table C.2: Character table for O_h.

(c) Matrices for irreducible representations of dimension greater than one, for any proper rotation C_{nj} of D_{6h}:

$$\begin{aligned}
\mathbf{\Gamma}^5(C_{nj}) &= \mathbf{\Gamma}^{11}(C_{nj}) &&= \mathbf{D}'(C_{nj});\\
\mathbf{\Gamma}^5(IC_{nj}) &= -\mathbf{\Gamma}^{11}(IC_{nj}) &&= \mathbf{D}'(C_{nj});\\
\mathbf{\Gamma}^6(C_{nj}) &= \mathbf{\Gamma}^{12}(C_{nj}) &&= \mathbf{D}''(C_{nj});\\
\mathbf{\Gamma}^6(IC_{nj}) &= -\mathbf{\Gamma}^{12}(IC_{nj}) &&= \mathbf{D}''(C_{nj});
\end{aligned}$$

where the matrices $\mathbf{D}'(C_{nj})$ and $\mathbf{D}''(C_{nj})$ are given in Tables C.6 and C.7 respectively.

(3) T_d:

(a) Classes [for $\mathcal{G}_0(\mathbf{k})$ of P]:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{3\alpha}, C_{3\beta}, C_{3\gamma}, C_{3\delta}, C_{3\alpha}^{-1}, C_{3\beta}^{-1}, C_{3\gamma}^{-1}, C_{3\delta}^{-1}$;
$\mathcal{C}_3 = C_{2x}, C_{2y}, C_{2z}$; $\mathcal{C}_4 = IC_{4x}, IC_{4y}, IC_{4z}, IC_{4x}^{-1}, IC_{4y}^{-1}, IC_{4z}^{-1}$;
$\mathcal{C}_5 = IC_{2a}, IC_{2b}, IC_{2c}, IC_{2d}, IC_{2e}, IC_{2f}$.

(b) The character table is given in Table C.8.

(c) Matrices for irreducible representations of dimension greater than one, for any proper rotation C_{nj} of T_d:

$$\mathbf{\Gamma}^3(C_{nj}) = \mathbf{\Gamma}''(C_{nj});\ \mathbf{\Gamma}^4(C_{nj}) = \mathbf{R}(C_{nj});\ \mathbf{\Gamma}^5(C_{nj}) = \mathbf{\Gamma}'(C_{nj});$$

and for any improper rotation IC_{nj} of T_d:

$$\mathbf{\Gamma}^3(IC_{nj}) = -\mathbf{\Gamma}''(C_{nj});\ \mathbf{\Gamma}^4(IC_{nj}) = -\mathbf{R}(C_{nj});$$

$$\mathbf{\Gamma}^5(IC_{nj}) = -\mathbf{\Gamma}'(C_{nj});$$

where the matrices $\mathbf{\Gamma}'(C_{nj})$, $\mathbf{\Gamma}''(C_{nj})$ and $\mathbf{R}(C_{nj})$ are given in Tables C.3, C.4, and C.1.

$$\Gamma'(E) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \Gamma'(C_{2x}) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix},$$

$$\Gamma'(C_{2y}) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \Gamma'(C_{2z}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix},$$

$$\Gamma'(C_{4x}) = \begin{bmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{bmatrix}, \quad \Gamma'(C_{4x}^{-1}) = \begin{bmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{bmatrix},$$

$$\Gamma'(C_{4y}) = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \quad \Gamma'(C_{4y}^{-1}) = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix},$$

$$\Gamma'(C_{4z}) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}, \quad \Gamma'(C_{4z}^{-1}) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix},$$

$$\Gamma'(C_{2a}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix}, \quad \Gamma'(C_{2b}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix},$$

$$\Gamma'(C_{2c}) = \begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \Gamma'(C_{2d}) = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

$$\Gamma'(C_{2e}) = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix}, \quad \Gamma'(C_{2f}) = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix},$$

$$\Gamma'(C_{3\alpha}) = \begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{bmatrix}, \quad \Gamma'(C_{3\beta}) = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{bmatrix},$$

$$\Gamma'(C_{3\gamma}) = \begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{bmatrix}, \quad \Gamma'(C_{3\delta}) = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix},$$

$$\Gamma'(C_{3\alpha}^{-1}) = \begin{bmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \quad \Gamma'(C_{3\beta}^{-1}) = \begin{bmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{bmatrix},$$

$$\Gamma'(C_{3\gamma}^{-1}) = \begin{bmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{bmatrix}, \quad \Gamma'(C_{3\delta}^{-1}) = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}.$$

Table C.3: The matrices Γ' for the proper rotations of O_h, T_d, O, T_h, and T.

$$\Gamma''(E) = \Gamma''(C_{2x}) = \Gamma''(C_{2y}) = \Gamma''(C_{2z}) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},$$

$$\Gamma''(C_{3\alpha}) = \Gamma''(C_{3\beta}) = \Gamma''(C_{3\gamma}) = \Gamma''(C_{3\delta}) = \begin{bmatrix} -\frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{bmatrix},$$

$$\Gamma''(C_{3\alpha}^{-1}) = \Gamma''(C_{3\beta}^{-1}) = \Gamma''(C_{3\gamma}^{-1}) = \Gamma''(C_{3\delta}^{-1}) = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{bmatrix},$$

$$\Gamma''(C_{4x}) = \Gamma''(C_{4x}^{-1}) = \Gamma''(C_{2e}) = \Gamma''(C_{2f}) = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{bmatrix},$$

$$\Gamma''(C_{4y}) = \Gamma''(C_{4y}^{-1}) = \Gamma''(C_{2c}) = \Gamma''(C_{2d}) = \begin{bmatrix} \frac{1}{2} & \frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{bmatrix},$$

$$\Gamma''(C_{4z}) = \Gamma''(C_{4z}^{-1}) = \Gamma''(C_{2a}) = \Gamma''(C_{2b}) = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}.$$

Table C.4: The matrices Γ'' for the proper rotations of O_h, T_d, O, T_h, and T.

		$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$	$\mathcal{C}_4$	$\mathcal{C}_5$	$\mathcal{C}_6$	$\mathcal{C}_7$	$\mathcal{C}_8$	$\mathcal{C}_9$	$\mathcal{C}_{10}$	$\mathcal{C}_{11}$	$\mathcal{C}_{12}$
Γ^1	A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1
Γ^2	A_{2g}	1	1	1	1	-1	-1	1	1	1	1	-1	-1
Γ^3	B_{1g}	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1
Γ^4	B_{2g}	1	-1	1	-1	-1	1	1	-1	1	-1	-1	1
Γ^5	E_{2g}	2	-1	-1	2	0	0	2	-1	-1	2	0	0
Γ^6	E_{1g}	2	1	-1	-2	0	0	2	1	-1	-2	0	0
Γ^7	A_{1u}	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1
Γ^8	A_{2u}	1	1	1	1	-1	-1	-1	-1	-1	-1	1	1
Γ^9	B_{1u}	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1
Γ^{10}	B_{2u}	1	-1	1	-1	-1	1	-1	1	-1	1	1	-1
Γ^{11}	E_{2u}	2	-1	-1	2	0	0	-2	1	1	-2	0	0
Γ^{12}	E_{1u}	2	1	-1	-2	0	0	-2	-1	1	2	0	0

Table C.5: Character table for D_{6h}.

$$\mathbf{D}'(E) = \mathbf{D}'(C_{2z}) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},$$

$$\mathbf{D}'(C_{6z}) = \mathbf{D}'(C_{3z}^{-1}) = \begin{bmatrix} -\frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{bmatrix},$$

$$\mathbf{D}'(C_{6z}^{-1}) = \mathbf{D}'(C_{3z}) = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{bmatrix},$$

$$\mathbf{D}'(C_{2x}) = \mathbf{D}'(C_{2y}) = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix},$$

$$\mathbf{D}'(C_{2A}) = \mathbf{D}'(C_{2C}) = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{bmatrix},$$

$$\mathbf{D}'(C_{2B}) = \mathbf{D}'(C_{2D}) = \begin{bmatrix} \frac{1}{2} & \frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{bmatrix}.$$

Table C.6: The matrices $\mathbf{D}'$ for the proper rotations of D_{6h}, D_{3h}, C_{6v}, and D_6.

$$\mathbf{D}''(E) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \qquad \mathbf{D}''(C_{6z}) = \begin{bmatrix} \frac{1}{2} & \frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & \frac{1}{2} \end{bmatrix},$$

$$\mathbf{D}''(C_{6z}^{-1}) = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & \frac{1}{2} \end{bmatrix}, \qquad \mathbf{D}''(C_{3z}) = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{bmatrix},$$

$$\mathbf{D}''(C_{3z}^{-1}) = \begin{bmatrix} -\frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{bmatrix}, \qquad \mathbf{D}''(C_{2z}) = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix},$$

$$\mathbf{D}''(C_{2x}) = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \qquad \mathbf{D}''(C_{2A}) = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & \frac{1}{2} \end{bmatrix},$$

$$\mathbf{D}''(C_{2B}) = \begin{bmatrix} -\frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & \frac{1}{2} \end{bmatrix}, \qquad \mathbf{D}''(C_{2y}) = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix},$$

$$\mathbf{D}''(C_{2C}) = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{bmatrix}, \qquad \mathbf{D}''(C_{2D}) = \begin{bmatrix} \frac{1}{2} & \frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{bmatrix}.$$

Table C.7: The matrices $\mathbf{D}''$ for the proper rotations of D_{6h}, C_{6v}, D_6 and D_3.

			$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$	$\mathcal{C}_4$	$\mathcal{C}_5$
$\mathbf{\Gamma}^1$	A_1	P_1	1	1	1	1	1
$\mathbf{\Gamma}^2$	A_2	P_2	1	1	1	−1	−1
$\mathbf{\Gamma}^3$	E	P_3	2	−1	2	0	0
$\mathbf{\Gamma}^4$	T_2	P_4	3	0	−1	−1	1
$\mathbf{\Gamma}^5$	T_1	P_5	3	0	−1	1	−1

Table C.8: Character table for T_d and O.

(4) O:

(a) Classes:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{3\alpha}, C_{3\beta}, C_{3\gamma}, C_{3\delta}, C_{3\alpha}^{-1}, C_{3\beta}^{-1}, C_{3\gamma}^{-1}, C_{3\delta}^{-1}$;
$\mathcal{C}_3 = C_{2x}, C_{2y}, C_{2z}$; $\mathcal{C}_4 = C_{4x}, C_{4y}, C_{4z}, C_{4x}^{-1}, C_{4y}^{-1}, C_{4z}^{-1}$;
$\mathcal{C}_5 = C_{2a}, C_{2b}, C_{2c}, C_{2d}, C_{2e}, C_{2f}$.

(b) The character table is given in Table C.8.

(c) Matrices for irreducible representations of dimension greater than one, for any proper rotation C_{nj} of O:

$$\mathbf{\Gamma}^3(C_{nj}) = \mathbf{\Gamma}''(C_{nj});\ \mathbf{\Gamma}^4(C_{nj}) = \mathbf{\Gamma}'(C_{nj});\ \mathbf{\Gamma}^5(C_{nj}) = \mathbf{R}(C_{nj});$$

where the matrices $\mathbf{\Gamma}'(C_{nj})$, $\mathbf{\Gamma}''(C_{nj})$ and $\mathbf{R}(C_{nj})$ are given in Tables C.3, C.4, and C.1.

(5) T_h:

(a) Classes:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{3\alpha}, C_{3\beta}, C_{3\gamma}, C_{3\delta}$; $\mathcal{C}_3 = C_{3\alpha}^{-1}, C_{3\beta}^{-1}, C_{3\gamma}^{-1}, C_{3\delta}^{-1}$;
$\mathcal{C}_4 = C_{2x}, C_{2y}, C_{2z}$; $\mathcal{C}_5 = I$; $\mathcal{C}_6 = IC_{3\alpha}, IC_{3\beta}, IC_{3\gamma}, IC_{3\delta}$;
$\mathcal{C}_7 = IC_{3\alpha}^{-1}, IC_{3\beta}^{-1}, IC_{3\gamma}^{-1}, IC_{3\delta}^{-1}$; $\mathcal{C}_8 = IC_{2x}, IC_{2y}, IC_{2z}$.

(b) The character table is given in Table C.9.

(c) Matrices for irreducible representations of dimension greater than one, for any proper rotation C_{nj} of T_h:

$$\mathbf{\Gamma}^4(C_{nj}) = \mathbf{\Gamma}^8(C_{nj}) = \mathbf{\Gamma}'(C_{nj});$$

$$\mathbf{\Gamma}^4(IC_{nj}) = -\mathbf{\Gamma}^8(IC_{nj}) = \mathbf{\Gamma}'(C_{nj});$$

where the matrices $\mathbf{\Gamma}'(C_{nj})$ are given in Table C.3.

		$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$	$\mathcal{C}_4$	$\mathcal{C}_5$	$\mathcal{C}_6$	$\mathcal{C}_7$	$\mathcal{C}_8$
Γ^1	A_g	1	1	1	1	1	1	1	1
Γ^2	E_g	1	ϕ	ϕ^2	1	1	ϕ	ϕ^2	1
Γ^3	E_g	1	ϕ^2	ϕ	1	1	ϕ^2	ϕ	1
Γ^4	T_g	3	0	0	-1	3	0	0	-1
Γ^5	A_u	1	1	1	1	-1	-1	-1	-1
Γ^6	E_u	1	ϕ	ϕ^2	1	-1	$-\phi$	$-\phi^2$	-1
Γ^7	E_u	1	ϕ^2	ϕ	1	-1	$-\phi^2$	$-\phi$	-1
Γ^8	T_u	3	0	0	-1	-3	0	0	1

Table C.9: Character table for T_h ($\phi = \exp(\frac{2}{3}\pi i)$).

			$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$	$\mathcal{C}_4$	$\mathcal{C}_5$	$\mathcal{C}_6$	$\mathcal{C}_7$	$\mathcal{C}_8$	$\mathcal{C}_9$	$\mathcal{C}_{10}$
Γ^1	A_{1g}	X_1, M_1	1	1	1	1	1	1	1	1	1	1
Γ^2	B_{1g}	X_2, M_2	1	1	1	-1	-1	1	1	1	-1	-1
Γ^3	B_{2g}	X_3, M_3	1	-1	1	-1	1	1	-1	1	-1	1
Γ^4	A_{2g}	X_4, M_4	1	-1	1	1	-1	1	-1	1	1	-1
Γ^5	E_g	X_5, M_5	2	0	-2	0	0	2	0	-2	0	0
Γ^6	A_{1u}	$X_{1'}, M_{1'}$	1	1	1	1	1	-1	-1	-1	-1	-1
Γ^7	B_{1u}	$X_{2'}, M_{2'}$	1	1	1	-1	-1	-1	-1	-1	1	1
Γ^8	B_{2u}	$X_{3'}, M_{3'}$	1	-1	1	-1	1	-1	1	-1	1	-1
Γ^9	A_{2u}	$X_{4'}, M_{4'}$	1	-1	1	1	-1	-1	1	-1	-1	1
Γ^{10}	E_u	$X_{5'}, M_{5'}$	2	0	-2	0	0	-2	0	2	0	0

Table C.10: Character table for D_{4h}.

(6) D_{4h}:

(a) (i) Classes [for $\mathcal{G}_0(\mathbf{k})$ of X]:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{2x}, C_{2y}$; $\mathcal{C}_3 = C_{2z}$; $\mathcal{C}_4 = C_{4z}, C_{4z}^{-1}$;
$\mathcal{C}_5 = C_{2a}, C_{2b}$; $\mathcal{C}_6 = I$; $\mathcal{C}_7 = IC_{2x}, IC_{2y}$; $\mathcal{C}_8 = IC_{2z}$;
$\mathcal{C}_9 = IC_{4z}, IC_{4z}^{-1}$; $\mathcal{C}_{10} = IC_{2a}, IC_{2b}$.

(ii) Classes [for $\mathcal{G}_0(\mathbf{k})$ of M]:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{2y}, C_{2z}$; $\mathcal{C}_3 = C_{2x}$; $\mathcal{C}_4 = C_{4x}, C_{4x}^{-1}$;
$\mathcal{C}_5 = C_{2e}, C_{2f}$; $\mathcal{C}_6 = I$; $\mathcal{C}_7 = IC_{2y}, IC_{2z}$; $\mathcal{C}_8 = IC_{2x}$;
$\mathcal{C}_9 = IC_{4x}, IC_{4x}^{-1}$; $\mathcal{C}_{10} = IC_{2e}, IC_{2f}$.

(b) The character table is given in Table C.10.

(c) Matrices for irreducible representations of dimension greater than one, for any proper rotation C_{nj} of D_{4h}:

$$\mathbf{\Gamma}^5(C_{nj}) = \mathbf{\Gamma}^{10}(C_{nj}) = \mathbf{D}(C_{nj});$$

$$\mathbf{\Gamma}^5(IC_{nj}) = -\mathbf{\Gamma}^{10}(IC_{nj}) = \mathbf{D}(C_{nj});$$

where for $\mathcal{G}_0(\mathbf{k})$ of M the matrices $\mathbf{D}(C_{nj})$ are given in Table C.11, while for $\mathcal{G}_0(\mathbf{k})$ of X the matrices $\mathbf{D}(C_{nj})$ are given in Table C.12.

$$\mathbf{D}(E) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \mathbf{D}(C_{2x}) = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \mathbf{D}(C_{2y}) = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},$$
$$\mathbf{D}(C_{2z}) = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \mathbf{D}(C_{4x}) = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad \mathbf{D}(C_{4x}^{-1}) = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix},$$
$$\mathbf{D}(C_{2e}) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \mathbf{D}(C_{2f}) = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}.$$

Table C.11: The matrices $\mathbf{D}$ for the proper rotations of D_{4h} for $\mathcal{G}_0(\mathbf{k})$ of M.

$$\mathbf{D}(E) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \mathbf{D}(C_{2x}) = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \mathbf{D}(C_{2y}) = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix},$$
$$\mathbf{D}(C_{2z}) = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \mathbf{D}(C_{4z}) = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad \mathbf{D}(C_{4z}^{-1}) = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix},$$
$$\mathbf{D}(C_{2a}) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \mathbf{D}(C_{2b}) = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}.$$

Table C.12: The matrices $\mathbf{D}$ for the proper rotations of D_{4h} for $\mathcal{G}_0(\mathbf{k})$ of X.

(7) D_{3h}:

(a) Classes:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{3z}, C_{3z}^{-1}$; $\mathcal{C}_3 = C_{2x}, C_{2A}, C_{2B}$;
$\mathcal{C}_4 = IC_{2z}$; $\mathcal{C}_5 = IC_{6z}, IC_{6z}^{-1}$; $\mathcal{C}_6 = IC_{2y}, IC_{2C}, IC_{2D}$.

(b) The character table is given in Table C.13.

(c) Matrices for irreducible representations of dimension greater than one, for any proper rotation C_{nj} of D_{3h}:

$$\mathbf{\Gamma}^3(C_{nj}) = \mathbf{\Gamma}^6(C_{nj}) = \mathbf{D}'(C_{nj});$$

and for any improper rotation IC_{nj} of D_{3h}:

$$\mathbf{\Gamma}^3(IC_{nj}) = -\mathbf{\Gamma}^6(IC_{nj}) = \mathbf{D}'(C_{nj});$$

where the matrices $\mathbf{D}'(C_{nj})$ are given in Table C.6.

(8) D_{3d}:

(a) Classes [for $\mathcal{G}_0(\mathbf{k})$ of L]:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{3\delta}, C_{3\delta}^{-1}$; $\mathcal{C}_3 = C_{2b}, C_{2d}, C_{2f}$;
$\mathcal{C}_4 = I$; $\mathcal{C}_5 = IC_{3\delta}, IC_{3\delta}^{-1}$; $\mathcal{C}_6 = IC_{2b}, IC_{2d}, IC_{2f}$.

(b) The character table is given in Table C.13.

	D_{3h}	D_{3d}	C_{6v}	D_6		$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$	$\mathcal{C}_4$	$\mathcal{C}_5$	$\mathcal{C}_6$
$\mathbf{\Gamma}^1$	A_1'	A_{1g}	A_1	A_1	L_1	1	1	1	1	1	1
$\mathbf{\Gamma}^2$	A_2'	A_{2g}	A_2	A_2	L_2	1	1	−1	1	1	−1
$\mathbf{\Gamma}^3$	E'	E_g	E_2	E_2	L_3	2	−1	0	2	−1	0
$\mathbf{\Gamma}^4$	A_1''	A_{1u}	B_1	B_1	$L_{1'}$	1	1	1	−1	−1	−1
$\mathbf{\Gamma}^5$	A_2''	A_{2u}	B_2	B_2	$L_{2'}$	1	1	−1	−1	−1	1
$\mathbf{\Gamma}^6$	E''	E_u	E_1	E_1	$L_{3'}$	2	−1	0	−2	1	0

Table C.13: Character table for D_{3h}, D_{3d}, C_{6v} and D_6.

(c) Matrices for irreducible representations of dimension greater than one, for any proper rotation C_{nj} of D_{3d}:

$$\mathbf{\Gamma}^3(C_{nj}) = \mathbf{\Gamma}^6(C_{nj}) = \mathbf{D}''(C_{nj});$$

$$\mathbf{\Gamma}^3(IC_{nj}) = -\mathbf{\Gamma}^6(IC_{nj}) = \mathbf{D}''(C_{nj});$$

where the matrices $\mathbf{D}''(C_{nj})$ are given in Table C.4.

(9) C_{6v}:

(a) Classes:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{3z}, C_{3z}^{-1}$; $\mathcal{C}_3 = IC_{2x}, IC_{2A}, IC_{2B}$;
$\mathcal{C}_4 = C_{2z}$; $\mathcal{C}_5 = C_{6z}, C_{6z}^{-1}$; $\mathcal{C}_6 = IC_{2y}, IC_{2C}, IC_{2D}$.

(b) The character table is given in Table C.13.

(c) Matrices for irreducible representations of dimension greater than one, for any proper rotation C_{nj} of C_{6v}:

$$\mathbf{\Gamma}^6(C_{nj}) = \mathbf{D}''(C_{nj});\ \mathbf{\Gamma}^3(C_{nj}) = \mathbf{D}'(C_{nj});$$

and for any improper rotation IC_{nj} of C_{6v}:

$$\mathbf{\Gamma}^6(IC_{nj}) = \mathbf{D}''(C_{nj});\ \mathbf{\Gamma}^3(IC_{nj}) = \mathbf{D}'(C_{nj});$$

where the matrices $\mathbf{D}'(C_{nj})$ and $\mathbf{D}''(C_{nj})$ are given in Tables C.6 and C.7 respectively.

(10) C_{6h}:

(a) Classes:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{6z}$; $\mathcal{C}_3 = C_{3z}$; $\mathcal{C}_4 = C_{2z}$; $\mathcal{C}_5 = C_{3z}^{-1}$; $\mathcal{C}_6 = C_{6z}^{-1}$;
$\mathcal{C}_7 = I$; $\mathcal{C}_8 = IC_{6z}$; $\mathcal{C}_9 = IC_{3z}$; $\mathcal{C}_{10} = IC_{2z}$; $\mathcal{C}_{11} = IC_{3z}^{-1}$;
$\mathcal{C}_{12} = IC_{6z}^{-1}$.

(b) The character table is given in Table C.14.

		$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$	$\mathcal{C}_4$	$\mathcal{C}_5$	$\mathcal{C}_6$	$\mathcal{C}_7$	$\mathcal{C}_8$	$\mathcal{C}_9$	$\mathcal{C}_{10}$	$\mathcal{C}_{11}$	$\mathcal{C}_{12}$
Γ^1	A_g	1	1	1	1	1	1	1	1	1	1	1	1
Γ^2	B_g	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1
Γ^3	E'_g	1	ω	ω^2	-1	$-\omega$	$-\omega^2$	1	ω	ω^2	-1	$-\omega$	$-\omega^2$
Γ^4	E'_g	1	$-\omega^2$	$-\omega$	-1	ω^2	ω	1	$-\omega^2$	$-\omega$	-1	ω^2	ω
Γ^5	E''_g	1	ω^2	$-\omega$	1	ω^2	$-\omega$	1	ω^2	$-\omega$	1	ω^2	$-\omega$
Γ^6	E''_g	1	$-\omega$	ω^2	1	$-\omega$	ω^2	1	$-\omega$	ω^2	1	$-\omega$	ω^2
Γ^7	A_u	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1
Γ^8	B_u	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1
Γ^9	E'_u	1	ω	ω^2	-1	$-\omega$	$-\omega^2$	-1	$-\omega$	$-\omega^2$	1	ω	ω^2
Γ^{10}	E'_u	1	$-\omega^2$	$-\omega$	-1	ω^2	ω	-1	ω^2	ω	1	$-\omega^2$	$-\omega$
Γ^{11}	E''_u	1	ω^2	$-\omega$	1	ω^2	$-\omega$	-1	$-\omega^2$	ω	-1	$-\omega^2$	ω
Γ^{12}	E''_u	1	$-\omega$	ω^2	1	$-\omega$	ω^2	-1	ω	$-\omega^2$	-1	ω	$-\omega^2$

Table C.14: Character table for C_{6h} ($\omega = \exp(\frac{1}{3}\pi i)$).

(11) D_6:

(a) Classes:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{3z}, C_{3z}^{-1}$; $\mathcal{C}_3 = C_{2x}, C_{2A}, C_{2B}$;
$\mathcal{C}_4 = C_{2z}$; $\mathcal{C}_5 = C_{6z}, C_{6z}^{-1}$; $\mathcal{C}_6 = C_{2y}, C_{2C}, C_{2D}$.

(b) The character table is given in Table C.13.

(c) Matrices for irreducible representations of dimension greater than one, for any proper rotation C_{nj} of C_{6v}:

$$\mathbf{\Gamma}^6(C_{nj}) = \mathbf{D}''(C_{nj}); \ \mathbf{\Gamma}^3(C_{nj}) = \mathbf{D}'(C_{nj});$$

where the matrices $\mathbf{D}'(C_{nj})$ and $\mathbf{D}''(C_{nj})$ are given in Tables C.6 and C.7 respectively.

(12) T:

(a) Classes:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{3\alpha}, C_{3\beta}, C_{3\gamma}, C_{3\delta}$; $\mathcal{C}_3 = C_{3\alpha}^{-1}, C_{3\beta}^{-1}, C_{3\gamma}^{-1}, C_{3\delta}^{-1}$;
$\mathcal{C}_4 = C_{2x}, C_{2y}, C_{2z}$.

(b) The character table is given in Table C.15.

(c) Matrices for irreducible representations of dimension greater than one, for any proper rotation C_{nj} of T:

$$\mathbf{\Gamma}^4(C_{nj}) = \mathbf{\Gamma}'(C_{nj});$$

where the matrices $\mathbf{\Gamma}'(C_{nj})$ are given in Tables C.3.

		$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$	$\mathcal{C}_4$
$\mathbf{\Gamma}^1$	A	1	1	1	1
$\mathbf{\Gamma}^2$	E	1	ϕ	ϕ^2	1
$\mathbf{\Gamma}^3$	E	1	ϕ^2	ϕ	1
$\mathbf{\Gamma}^4$	T	3	0	0	-1

Table C.15: Character table for T ($\phi = \exp(\frac{2}{3}\pi i)$).

			$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$	$\mathcal{C}_4$	$\mathcal{C}_5$	$\mathcal{C}_6$	$\mathcal{C}_7$	$\mathcal{C}_8$
$\mathbf{\Gamma}^1$	A_{1g}	N_1	1	1	1	1	1	1	1	1
$\mathbf{\Gamma}^2$	B_{1g}	N_2	1	-1	1	-1	1	-1	1	-1
$\mathbf{\Gamma}^3$	B_{2g}	N_3	1	-1	-1	1	1	-1	-1	1
$\mathbf{\Gamma}^4$	B_{3g}	N_4	1	1	-1	-1	1	1	-1	-1
$\mathbf{\Gamma}^5$	A_{1u}	$N_{2'}$	1	1	1	1	-1	-1	-1	-1
$\mathbf{\Gamma}^6$	B_{1u}	$N_{1'}$	1	-1	1	-1	-1	1	-1	1
$\mathbf{\Gamma}^7$	B_{2u}	$N_{4'}$	1	-1	-1	1	-1	1	1	-1
$\mathbf{\Gamma}^8$	B_{3u}	$N_{3'}$	1	1	-1	-1	-1	-1	1	1

Table C.16: Character table for D_{2h}.

(13) D_{2h} or V_h:

(a) Classes [for $\mathcal{G}_0(\mathbf{k})$ of N]:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{2x}$; $\mathcal{C}_3 = C_{2e}$; $\mathcal{C}_4 = C_{2f}$;
$\mathcal{C}_5 = I$; $\mathcal{C}_6 = IC_{2x}$; $\mathcal{C}_7 = IC_{2e}$; $\mathcal{C}_8 = IC_{2f}$.

(b) The character table is given in Table C.16.

(14) C_{4v}:

(a) Classes [for $\mathcal{G}_0(\mathbf{k})$ of Δ]:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{2z}$, $\mathcal{C}_3 = C_{4z}, C_{4z}^{-1}$; $\mathcal{C}_4 = IC_{2x}, IC_{2y}$; $\mathcal{C}_5 = IC_{2a}, IC_{2b}$.

(b) Classes [for $\mathcal{G}_0(\mathbf{k})$ of T]:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{2x}$, $\mathcal{C}_3 = C_{4x}, C_{4x}^{-1}$; $\mathcal{C}_4 = IC_{2y}, IC_{2z}$; $\mathcal{C}_5 = IC_{2e}, IC_{2f}$.

(c) The character table is given in Table C.17.

(d) Matrices for irreducible representations of dimension greater than one, for any proper rotation C_{nj} of C_{4v}:

$$\mathbf{\Gamma}^5(C_{nj}) = \mathbf{D}(C_{nj});$$

and for any improper rotation IC_{nj} of C_{4v}:

$$\mathbf{\Gamma}^5(IC_{nj}) = -\mathbf{D}(C_{nj});$$

where for $\mathcal{G}_0(\mathbf{k})$ of Δ the matrices $\mathbf{D}(C_{nj})$ are given in Table C.12 and for $\mathcal{G}_0(\mathbf{k})$ of T they are given in Table C.11.

				$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$	$\mathcal{C}_4$	$\mathcal{C}_5$
$\mathbf{\Gamma}^1$	A_1	Δ_1,T_1	W_1	1	1	1	1	1
$\mathbf{\Gamma}^2$	B_1	Δ_2,T_2	$W_{2'}$	1	1	−1	1	−1
$\mathbf{\Gamma}^3$	A_2	$\Delta_{1'}$,$T_{1'}$	W_2	1	1	1	−1	−1
$\mathbf{\Gamma}^4$	B_2	$\Delta_{2'}$,$T_{2'}$	$W_{1'}$	1	1	−1	−1	1
$\mathbf{\Gamma}^5$	E	Δ_5,T_5	W_3	2	−2	0	0	0

Table C.17: Character table for C_{4v}, D_4 and D_{2d}.

(15) D_4:

(a) Classes:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{2y}$; $\mathcal{C}_3 = C_{4y}, C_{4y}^{-1}$; $\mathcal{C}_4 = C_{2x}, C_{2z}$; $\mathcal{C}_5 = C_{2c}, C_{2d}$.

(b) The character table is given in Table C.17.

(c) Matrices for irreducible representations of dimension greater than one, for any proper rotation C_{nj} of D_4:

$$\mathbf{\Gamma}^5(C_{nj}) = \mathbf{S}(C_{nj});$$

where the matrices $\mathbf{S}(C_{nj})$ are given in Tables C.18.

(16) D_{2d} or V_d:

(a) Classes [for $\mathcal{G}_0(\mathbf{k})$ of W]:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{2y}$; $\mathcal{C}_3 = IC_{4y}, IC_{4y}^{-1}$; $\mathcal{C}_4 = IC_{2x}, IC_{2z}$; $\mathcal{C}_5 = C_{2c}, C_{2d}$.

(b) The character table is given in Table C.17.

(c) Matrices for irreducible representations of dimension greater than one, for any proper rotation C_{nj} of D_{2d}:

$$\mathbf{\Gamma}^5(C_{nj}) = \mathbf{S}(C_{nj});$$

and for any improper rotation IC_{nj} of D_{2d}:

$$\mathbf{\Gamma}^5(IC_{nj}) = -\mathbf{S}(C_{nj});$$

where the matrices $\mathbf{S}(C_{nj})$ are given in Tables C.18.

(17) C_{4h}:

(a) Classes:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{4z}$; $\mathcal{C}_3 = C_{2z}$; $\mathcal{C}_4 = C_{4z}^{-1}$;
$\mathcal{C}_5 = I$; $\mathcal{C}_6 = IC_{4z}$; $\mathcal{C}_7 = IC_{2z}$; $\mathcal{C}_8 = IC_{4z}^{-1}$.

(b) The character table is given in Table C.19.

$$\mathbf{S}(E) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \mathbf{S}(C_{2y}) = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \mathbf{S}(C_{2c}) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

$$\mathbf{S}(C_{2d}) = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}, \quad \mathbf{S}(C_{4y}) = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \quad \mathbf{S}(C_{4y}^{-1}) = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix},$$

$$\mathbf{S}(C_{2x}) = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \mathbf{S}(C_{2z}) = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}.$$

Table C.18: The matrices $\mathbf{S}$ for the proper rotations of D_4 and D_{2d}.

		$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$	$\mathcal{C}_4$	$\mathcal{C}_5$	$\mathcal{C}_6$	$\mathcal{C}_7$	$\mathcal{C}_8$
$\mathbf{\Gamma}^1$	A_g	1	1	1	1	1	1	1	1
$\mathbf{\Gamma}^2$	B_g	1	−1	1	−1	1	−1	1	−1
$\mathbf{\Gamma}^3$	E_g	1	i	−1	$-i$	1	i	−1	$-i$
$\mathbf{\Gamma}^4$	E_g	1	$-i$	−1	i	1	$-i$	−1	i
$\mathbf{\Gamma}^5$	A_u	1	1	1	1	−1	−1	−1	−1
$\mathbf{\Gamma}^6$	B_u	1	−1	1	−1	−1	1	−1	1
$\mathbf{\Gamma}^7$	E_u	1	i	−1	$-i$	−1	$-i$	1	i
$\mathbf{\Gamma}^8$	E_u	1	$-i$	−1	i	−1	i	1	$-i$

Table C.19: Character table for D_{4h}.

(18) C_{3h}:

(a) Classes:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = IC_{6z}$; $\mathcal{C}_3 = C_{3z}$; $\mathcal{C}_4 = IC_{2z}$; $\mathcal{C}_5 = C_{3z}^{-1}$; $\mathcal{C}_6 = IC_{6z}^{-1}$.

(b) The character table is given in Table C.20.

(19) C_{3v}:

(a) Classes [for $\mathcal{G}_0(\mathbf{k})$ of Λ]:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{3\delta}, C_{3\delta}^{-1}$; $\mathcal{C}_3 = IC_{2b}, IC_{2d}, IC_{2f}$.

(b) Classes [for $\mathcal{G}_0(\mathbf{k})$ of F]:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{3\alpha}, C_{3\alpha}^{-1}$; $\mathcal{C}_3 = IC_{2b}, IC_{2c}, IC_{2e}$.

	C_{3h}	C_{3i}	C_6	$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$	$\mathcal{C}_4$	$\mathcal{C}_5$	$\mathcal{C}_6$
$\mathbf{\Gamma}^1$	A'	A_g	A	1	1	1	1	1	1
$\mathbf{\Gamma}^2$	A''	A_u	B	1	−1	1	−1	1	−1
$\mathbf{\Gamma}^3$	E''	E_u	E'	1	ω	ω^2	−1	$-\omega$	$-\omega^2$
$\mathbf{\Gamma}^4$	E''	E_u	E'	1	$-\omega^2$	$-\omega$	−1	ω^2	ω
$\mathbf{\Gamma}^5$	E'	E_g	E''	1	ω^2	$-\omega$	1	ω^2	$-\omega$
$\mathbf{\Gamma}^6$	E'	E_g	E''	1	$-\omega$	ω^2	1	$-\omega$	ω^2

Table C.20: Character table for C_{3h}, C_{3i} and C_6 ($\omega = \exp(\frac{1}{3}\pi i)$).

			$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$
$\mathbf{\Gamma}^1$	A_1	F_1,Λ_1	1	1	1
$\mathbf{\Gamma}^2$	A_2	F_2,Λ_2	1	1	-1
$\mathbf{\Gamma}^3$	E	F_3,Λ_3	2	-1	0

Table C.21: Character table for C_{3v} and D_3.

(c) The character table is given in Table C.21.

(d) Matrices for irreducible representations of dimension greater than one, for any proper rotation C_{nj} of C_{3v}:

$$\mathbf{\Gamma}^3(C_{nj}) = \mathbf{\Gamma}''(C_{nj});$$

and for any improper rotation IC_{nj} of C_{3v}:

$$\mathbf{\Gamma}^3(IC_{nj}) = \mathbf{\Gamma}''(C_{nj});$$

where the matrices $\mathbf{\Gamma}''(C_{nj})$ are given in Tables C.4.

(20) D_3:

(a) Classes:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{3z}, C_{3z}^{-1}$; $\mathcal{C}_3 = C_{2x}, C_{2A}, C_{2B}$.

(b) The character table is given in Table C.21.

(c) Matrices for irreducible representations of dimension greater than one, for any proper rotation C_{nj} of D_3:

$$\mathbf{\Gamma}^3(C_{nj}) = \mathbf{D}'(C_{nj});$$

where the matrices $\mathbf{D}'(C_{nj})$ are given in Tables C.6.

(21) C_{3i} or S_6:

(a) Classes:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = IC_{3z}^{-1}$; $\mathcal{C}_3 = C_{3z}$, $\mathcal{C}_4 = I$, $\mathcal{C}_5 = C_{3z}^{-1}$, $\mathcal{C}_6 = IC_{3z}$.

(b) The character table is given in Table C.20.

	C_{2v}	C_{2h}	D_2						$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$	$\mathcal{C}_4$
$\mathbf{\Gamma}^1$	A_1	A_g	A_1	Σ_1	S_1	Z_1	G_1	D_1	1	1	1	1
$\mathbf{\Gamma}^2$	A_2	A_u	B_1	Σ_2	S_2	Z_2	G_2	D_2	1	1	−1	−1
$\mathbf{\Gamma}^3$	B_1	B_u	B_2	Σ_3	S_3	Z_3	G_3	D_3	1	−1	−1	1
$\mathbf{\Gamma}^4$	B_2	B_g	B_3	Σ_4	S_4	Z_4	G_4	D_4	1	−1	1	−1

Table C.22: Character table for C_{2v}, C_{2h} and D_2.

(22) C_6:

(a) Classes:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{6z}$; $\mathcal{C}_3 = C_{3z}$, $\mathcal{C}_4 = C_{2z}$, $\mathcal{C}_5 = C_{3z}^{-1}$, $\mathcal{C}_6 = C_{6z}^{-1}$.

(b) The character table is given in Table C.20.

(23) C_{2v}:

(a) Classes [for $\mathcal{G}_0(\mathbf{k})$ of Σ]:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{2e}$; $\mathcal{C}_3 = IC_{2x}$, $\mathcal{C}_4 = IC_{2f}$.
Classes [for $\mathcal{G}_0(\mathbf{k})$ of D]:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{2x}$; $\mathcal{C}_3 = IC_{2e}$, $\mathcal{C}_4 = IC_{2f}$.
Classes [for $\mathcal{G}_0(\mathbf{k})$ of S]:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{2a}$; $\mathcal{C}_3 = IC_{2z}$, $\mathcal{C}_4 = IC_{2b}$.
Classes [for $\mathcal{G}_0(\mathbf{k})$ of Z]:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{2y}$; $\mathcal{C}_3 = IC_{2z}$, $\mathcal{C}_4 = IC_{2x}$.
Classes [for $\mathcal{G}_0(\mathbf{k})$ of G]:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{2f}$; $\mathcal{C}_3 = IC_{2x}$, $\mathcal{C}_4 = IC_{2e}$.

(b) The character table is given in Table C.22.

(24) C_{2h}:

(a) Classes:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{2z}$; $\mathcal{C}_3 = I$, $\mathcal{C}_4 = IC_{2z}$.

(b) The character table is given in Table C.22.

(25) D_2 or V:

(a) Classes:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{2x}$; $\mathcal{C}_3 = C_{2y}$, $\mathcal{C}_4 = C_{2z}$.

(b) The character table is given in Table C.22.

(26) C_4:

(a) Classes:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{4z}$; $\mathcal{C}_3 = C_{2z}$, $\mathcal{C}_4 = C_{4z}^{-1}$.

		$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$	$\mathcal{C}_4$
$\mathbf{\Gamma}^1$	A	1	1	1	1
$\mathbf{\Gamma}^2$	B	1	-1	1	-1
$\mathbf{\Gamma}^3$	E	1	i	-1	$-i$
$\mathbf{\Gamma}^4$	E	1	$-i$	-1	i

Table C.23: Character table for C_4 and S_4.

		$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$
$\mathbf{\Gamma}^1$	A	1	1	1
$\mathbf{\Gamma}^2$	E	1	ϕ	ϕ^2
$\mathbf{\Gamma}^3$	E	1	ϕ^2	ϕ

Table C.24: Character table for C_3 ($\phi = \exp(\frac{2}{3}\pi i)$).

(b) The character table is given in Table C.23.

(27) S_4:

(a) Classes:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = IC_{4y}$; $\mathcal{C}_3 = C_{2y}$, $\mathcal{C}_4 = IC_{4y}^{-1}$.

(b) The character table is given in Table C.23.

(28) C_3:

(a) Classes:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{3z}$; $\mathcal{C}_3 = C_{3z}^{-1}$.

(b) The character table is given in Table C.24.

(29) C_s or C_{1h}:

(a) Classes:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = IC_{2z}$.

(b) The character table is given in Table C.25.

	C_s	C_2	C_i		$\mathcal{C}_1$	$\mathcal{C}_2$
$\mathbf{\Gamma}^1$	A'	A	A_g	Q_1	1	1
$\mathbf{\Gamma}^2$	A''	B	A_u	Q_2	1	-1

Table C.25: Character table for C_s, C_2 and C_i.

(30) C_2:

(a) Classes [for $\mathcal{G}_0(\mathbf{k})$ of Q]:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = C_{2d}$.

(b) The character table is given in Table C.25.

(31) C_i or S_2:

(a) Classes:
$\mathcal{C}_1 = E$; $\mathcal{C}_2 = I$.

(b) The character table is given in Table C.25.

(32) C_1:

(a) This group consists of E alone.

(b) $\chi(E) = 1$.

Appendix D

Properties of the Classical Simple Complex Lie Algebras

1 The simple complex Lie algebra A_l, $l \geq 1$

(a) The Dynkin diagram is given in Figure D.1.

(b) The Cartan matrix of A_l is

$$\mathbf{A} = \begin{bmatrix} 2 & -1 & 0 & \dots & 0 & 0 & 0 \\ -1 & 2 & -1 & \dots & 0 & 0 & 0 \\ 0 & -1 & 2 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 2 & -1 & 0 \\ 0 & 0 & 0 & \dots & -1 & 2 & -1 \\ 0 & 0 & 0 & \dots & 0 & -1 & 2 \end{bmatrix}.$$

(c) (i) A_l has $\frac{1}{2}l(l+1)$ positive roots, namely $\sum_{p=j}^{k} \alpha_p$ for all $j, k = 1, 2, \dots, l$ with $j \leq k$.

(ii) It is sometimes convenient to introduce $(l+1)$ auxiliary linear functionals $\epsilon_1, \epsilon_1, \dots, \epsilon_{l+1}$ on $\mathcal{H}$. In terms of these the positive

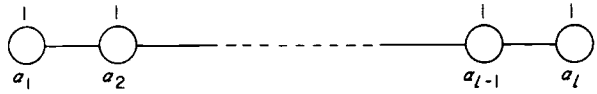

Figure D.1: The Dynkin diagram of A_l $(l = 1, 2, 3, \dots)$.

roots are $(\epsilon_p - \epsilon_q)$ $(p, q = 1, 2, \ldots, l+1;\ p < q)$, with $\alpha_j = \epsilon_j - \epsilon_{j+1}$ (for $j = 1, 2, \ldots, l$).

(d) The dimension n of A_l is given by $n = (l+1)^2 - 1$.

(e) The quantities $\langle \alpha_j, \alpha_k \rangle$ defined in Equation (11.10) are given for A_l by

$$\langle \alpha_j, \alpha_k \rangle = \begin{cases} 1/(l+1), & \text{for } j = k, (j = 1, 2, \ldots, l); \\ -1/\{2(l+1)\}, & \text{for } j = k \pm 1, (j, k = 1, 2, \ldots, l); \\ 0, & \text{for other values of } j, k, (j, k = 1, \ldots, l). \end{cases}$$

(f) The order of the Weyl group $\mathcal{W}$ for A_l is $(l+1)!$.

(g) The fundamental weights of A_l are

$$\Lambda_j = \begin{cases} \{1/(l+1)\} \sum_{p=1}^{l} (l+1-p)\alpha_p, \text{ for } j = 1; \\ \{1/(l+1)\}\{\sum_{p=1}^{j-1} p(l+1-p)\alpha_p + \sum_{p=j}^{l} j(l+1-p)\alpha_p\}, \\ \quad \text{for } j = 2, 3, \ldots, l, \end{cases}$$

as

$$\mathbf{A}^{-1} = \{1/(l+1)\} \times \begin{bmatrix} l & (l-1) & (l-2) & (l-3) & \ldots & 3 & 2 & 1 \\ (l-1) & 2(l-1) & 2(l-2) & 2(l-3) & \ldots & 6 & 4 & 2 \\ (l-2) & 2(l-2) & 3(l-2) & 3(l-3) & \ldots & 9 & 6 & 3 \\ (l-3) & 2(l-3) & 3(l-3) & 4(l-3) & \ldots & 12 & 8 & 4 \\ \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 3 & 6 & 9 & 12 & \ldots & 3(l-2) & 2(l-2) & (l-2) \\ 2 & 4 & 6 & 8 & \ldots & 2(l-2) & 2(l-1) & (l-1) \\ 1 & 2 & 3 & 4 & \ldots & (l-2) & (l-1) & l \end{bmatrix}.$$

(h) The compact real form of A_l is $\mathrm{su}(l+1)$.

(i) The adjoint representation is $\mathbf{\Gamma}(\{2\})$ for A_1 and $\mathbf{\Gamma}(\{1, 0, \ldots, 0, 1\})$ for A_l, $l > 1$.

2 The simple complex Lie algebra B_l, $l \geq 1$

(a) The Dynkin diagram is given in Figure D.2.

(b) The Cartan matrix of B_l is

$$\mathbf{A} = \begin{bmatrix} 2 & -1 & 0 & \ldots & 0 & 0 & 0 \\ -1 & 2 & -1 & \ldots & 0 & 0 & 0 \\ 0 & -1 & 2 & \ldots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & 2 & -1 & 0 \\ 0 & 0 & 0 & \ldots & -1 & 2 & -1 \\ 0 & 0 & 0 & \ldots & 0 & -2 & 2 \end{bmatrix}.$$

In particular, for $l = 2$ and $l = 3$ respectively

$$\mathbf{A} = \begin{bmatrix} 2 & -1 \\ -2 & 2 \end{bmatrix} \text{ and } \mathbf{A} = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -2 & 2 \end{bmatrix}.$$

(c) (i) B_l has l^2 positive roots, namely

$$\left.\begin{array}{ll} \sum_{p=j}^{l} \alpha_p, & \text{for } j = 1, 2, \ldots, l; \\ \sum_{p=j}^{k-1} \alpha_p + 2\sum_{p=k}^{l} \alpha_p, & \text{for } j, k = 1, 2, \ldots, l;\ j < k; \\ \sum_{p=j}^{k-1} \alpha_p, & \text{for } j, k = 1, 2, \ldots, l;\ j < k. \end{array}\right\}$$

(ii) It is sometimes convenient to introduce l auxiliary linear functionals $\epsilon_1, \epsilon_1, \ldots, \epsilon_l$ on $\mathcal{H}$, with $\alpha_j = \epsilon_j - \epsilon_{j+1}$ (for $j = 1, 2, \ldots, l-1$) and $\alpha_l = \epsilon_l$. The pattern of positive roots then appears more regular, as it consists of

$$\epsilon_j \ (j = 1, 2, \ldots, l) \text{ and } (\epsilon_j \pm \epsilon_k) \ (j, k = 1, 2, \ldots, l;\ j < k).$$

(d) The dimension n of B_l is given by $n = l(2l + 1)$.

(e) The quantities $\langle \alpha_j, \alpha_k \rangle$ (as defined in Equation (11.10)) are given for B_l by

$$\langle \alpha_j, \alpha_k \rangle = \begin{cases} 1/(2l-1), & \text{for } j = k, (j = 1, 2, \ldots, l-1); \\ 1/\{2(2l-1)\}, & \text{for } j = k = l; \\ -1/\{2(2l-1)\}, & \text{for } j = k \pm 1, (j, k = 1, 2, \ldots, l); \\ 0, & \text{for all other } j, k, (j, k = 1, \ldots, l). \end{cases}$$

(f) The order of the Weyl group $\mathcal{W}$ for B_l is $2^l l!$.

(g) The fundamental weights of B_l are

$$\Lambda_j = \begin{cases} \sum_{p=1}^{l} \alpha_p, & \text{for } j = 1; \\ \sum_{p=1}^{j-1} p\alpha_p + \sum_{p=j}^{l} j\alpha_p, & \text{for } j = 2, 3, \ldots, l-1; \\ \frac{1}{2}\sum_{p=1}^{l} p\alpha_p, & \text{for } j = l; \end{cases}$$

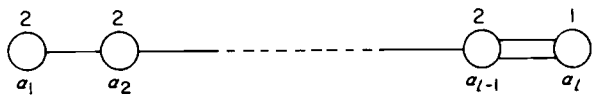

Figure D.2: The Dynkin diagram of B_l $(l = 1, 2, 3, \ldots)$.

as

$$\mathbf{A}^{-1} = \begin{bmatrix} 1 & 1 & 1 & 1 & \dots & 1 & 1 & \frac{1}{2} \\ 1 & 2 & 2 & 2 & \dots & 2 & 2 & 1 \\ 1 & 2 & 3 & 3 & \dots & 3 & 3 & \frac{3}{2} \\ 1 & 2 & 3 & 4 & \dots & 4 & 4 & 2 \\ \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 1 & 2 & 3 & 4 & \dots & (l-2) & (l-2) & \frac{1}{2}(l-2) \\ 1 & 2 & 3 & 4 & \dots & (l-2) & (l-1) & \frac{1}{2}(l-1) \\ 1 & 2 & 3 & 4 & \dots & (l-2) & (l-1) & \frac{1}{2}l \end{bmatrix}.$$

(h) The compact real form of B_l is $\mathrm{so}(2l+1)$.

(i) The adjoint representation is $\mathbf{\Gamma}(\{2\})$ for B_1 and $\mathbf{\Gamma}(\{0,1,0,\dots,0\})$ for B_l for $l > 1$.

3 The simple complex Lie algebra C_l, $l \geq 1$

(a) The Dynkin diagram is given in Figure D.3.

(b) The Cartan matrix of C_l is

$$\mathbf{A} = \begin{bmatrix} 2 & -1 & 0 & \dots & 0 & 0 & 0 \\ -1 & 2 & -1 & \dots & 0 & 0 & 0 \\ 0 & -1 & 2 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 2 & -1 & 0 \\ 0 & 0 & 0 & \dots & -1 & 2 & -2 \\ 0 & 0 & 0 & \dots & 0 & -1 & 2 \end{bmatrix}.$$

In particular, for $l = 2$ and $l = 3$ respectively

$$\mathbf{A} = \begin{bmatrix} 2 & -2 \\ -1 & 2 \end{bmatrix} \text{ and } \mathbf{A} = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -2 \\ 0 & -1 & 2 \end{bmatrix}.$$

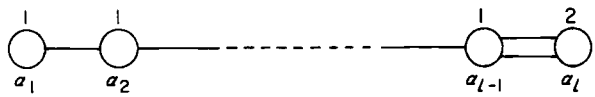

Figure D.3: The Dynkin diagram of C_l ($l = 1, 2, 3, \dots$).

(c) (i) C_l has l^2 positive roots, namely

$$\left.\begin{array}{ll} \sum_{p=j}^{k-1}\alpha_p, & \text{for } j,k=1,2,\ldots,l;\ j<k; \\ \sum_{p=j}^{k-1}\alpha_p+2\sum_{p=k}^{l-1}\alpha_p+\alpha_l, & \text{for } j,k=1,2,\ldots,l-1;\ j<k; \\ \sum_{p=j}^{l-1}\alpha_p+\alpha_l, & \text{for } j=1,2,\ldots,l-1; \\ 2\sum_{p=j}^{l-1}\alpha_p+\alpha_l, & \text{for } j=1,2,\ldots,l-1; \\ \alpha_l. & \end{array}\right\}$$

(ii) It is sometimes convenient to introduce l auxiliary linear functionals $\epsilon_1,\epsilon_1,\ldots,\epsilon_l$ on $\mathcal{H}$, with $\alpha_j=\epsilon_j-\epsilon_{j+1}$ (for $j=1,2,\ldots,l-1$) and $\alpha_l=2\epsilon_l$. The pattern of positive roots then appears more regular, as it consists of

$$\left.\begin{array}{ll} (\epsilon_j-\epsilon_k), & (j,k=1,2,\ldots,l;\ j<k); \\ (\epsilon_j+\epsilon_k), & (j,k=1,2,\ldots,l;\ j\le k). \end{array}\right\}$$

(d) The dimension n of C_l is given by $n=l(2l+1)$.

(e) The quantities $\langle\alpha_j,\alpha_k\rangle$ (as defined in Equation (11.10)) are given for C_l by

$$\langle\alpha_j,\alpha_k\rangle=\begin{cases} 1/\{2(l+1)\}, & \text{for } j=k,(j=1,2,\ldots,l-1); \\ 1/(l+1), & \text{for } j=k=l; \\ -1/\{4(l+1)\}, & \text{for } j=k\pm1,(j,k=1,2,\ldots,l-1); \\ -1/\{2(l+1)\}, & \text{for } j=l-1,k=l,\ \&\ j=l,k=l-1; \\ 0, & \text{for all other } j,k,(j,k=1,\ldots,l). \end{cases}$$

(f) The order of the Weyl group $\mathcal{W}$ for C_l is $2^l l!$.

(g) The fundamental weights of C_l are

$$\Lambda_j=\begin{cases} \sum_{p=1}^{l-1}\alpha_p+\frac{1}{2}\alpha_l, & \text{for } j=1; \\ \sum_{p=1}^{j-1}p\alpha_p+\sum_{p=j}^{l-1}j\alpha_p+\frac{1}{2}j\alpha_l, & \text{for } j=2,3,\ldots,l-1; \\ \sum_{p=1}^{l-1}p\alpha_p+\frac{1}{2}l\alpha_l, & \text{for } j=l; \end{cases}$$

as

$$\mathbf{A}^{-1}=\begin{bmatrix} 1 & 1 & 1 & 1 & \ldots & 1 & 1 & 1 \\ 1 & 2 & 2 & 2 & \ldots & 2 & 2 & 2 \\ 1 & 2 & 3 & 3 & \ldots & 3 & 3 & 3 \\ 1 & 2 & 3 & 4 & \ldots & 4 & 4 & 4 \\ \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 1 & 2 & 3 & 4 & \ldots & (l-2) & (l-2) & (l-2) \\ 1 & 2 & 3 & 4 & \ldots & (l-2) & (l-1) & (l-1) \\ \frac{1}{2} & 1 & \frac{3}{2} & 2 & \ldots & \frac{1}{2}(l-2) & \frac{1}{2}(l-1) & \frac{1}{2}l \end{bmatrix}.$$

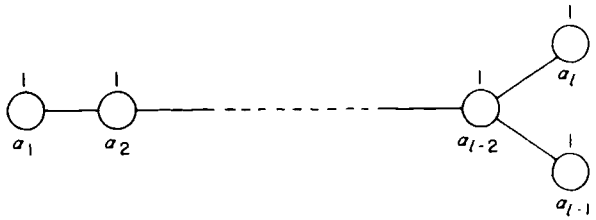

Figure D.4: The Dynkin diagram of D_l ($l = 3, 4, 5, \ldots$).

Figure D.5: The Dynkin diagram of D_2.

(h) The compact real form of C_l is $\mathrm{sp}(l)$.

(i) The adjoint representation is $\mathbf{\Gamma}(\{2, 0, \ldots, 0\})$.

4 The simple complex Lie algebra D_l, $l \geq 3$ (and the semi-simple complex Lie algebra D_2)

(a) The Dynkin diagram for D_l for $l \geq 3$ is given in Figure D.4 and the corresponding diagram for D_2 is given in Figure D.5.

(b) The Cartan matrix of D_l is

$$\mathbf{A} = \begin{bmatrix} 2 & -1 & 0 & \ldots & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & \ldots & 0 & 0 & 0 & 0 \\ 0 & -1 & 2 & \ldots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & \ldots & -1 & 2 & -1 & -1 \\ 0 & 0 & 0 & \ldots & 0 & -1 & 2 & 0 \\ 0 & 0 & 0 & \ldots & 0 & -1 & 0 & 2 \end{bmatrix}.$$

In particular, for $l = 3$ and $l = 4$ respectively

$$\mathbf{A} = \begin{bmatrix} 2 & -1 & -1 \\ -1 & 2 & 0 \\ -1 & 0 & 2 \end{bmatrix} \text{ and } \mathbf{A} = \begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & -1 \\ 0 & -1 & 2 & 0 \\ 0 & -1 & 0 & 2 \end{bmatrix}.$$

For $l = 2$

$$\mathbf{A} = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}.$$

(c) (i) D_l has $l(l-1)$ positive roots, namely

(1) for $j, k = 1, 2, \ldots, l-2$; $j < k$; $(l \geq 3)$:

$$\left.\begin{array}{l} \sum_{p=j}^{k-1} \alpha_p + 2\sum_{p=k}^{l-2} \alpha_p + \alpha_{l-1} + \alpha_l, \\ \sum_{p=j}^{k-1} \alpha_p, \end{array}\right\}$$

(2) for $j = 1, 2, \ldots, l-2$; $j < k$; $(l \geq 3)$:

$$\left.\begin{array}{l} \sum_{p=j}^{l-2} \alpha_p + \alpha_{l-1} + \alpha_l, \\ \sum_{p=j}^{l-2} \alpha_p + \alpha_{l-1}, \\ \sum_{p=j}^{l-2} \alpha_p + \alpha_l, \\ \sum_{p=j}^{l-2} \alpha_p, \end{array}\right\}$$

(3) α_{l-1} and α_l.

(ii) It is sometimes convenient to introduce l auxiliary linear functionals $\epsilon_1, \epsilon_1, \ldots, \epsilon_l$ on $\mathcal{H}$, with $\alpha_j = \epsilon_j - \epsilon_{j+1}$ (for $j = 1, 2, \ldots, l-1$) and $\alpha_l = \epsilon_{l-1} + \epsilon_l$. The pattern of positive roots then appears more regular, as it consists of $(\epsilon_j \pm \epsilon_k)$ for $j, k = 1, 2, \ldots, l$ with $j < k$).

(d) The dimension n of D_l is given by $n = l(2l-1)$.

(e) The quantities $\langle \alpha_j, \alpha_k \rangle$ (as defined in Equation (11.10)) are given for D_l by

$$\langle \alpha_j, \alpha_k \rangle = \begin{cases} 1/\{2(l-1)\}, & \text{for } j = k, (j = 1, 2, \ldots, l); \\ -1/\{4(l-1)\}, & \text{for } j = k \pm 1, (j, k = 1, 2, \ldots, l-3); \\ & \text{and for } j = l-2 \text{ with } k = l-1, l; \\ & \text{and for } k = l-2 \text{ with } j = l-1, l; \\ & \text{(all for } l \geq 3) \\ 0, & \text{for all other } j, k, (j, k = 1, \ldots, l). \end{cases}$$

(f) The order of the Weyl group $\mathcal{W}$ for D_l is $2^{l-1} l!$.

(g) The fundamental weights of D_l are

$$\Lambda_j = \begin{cases} \sum_{p=1}^{l-2} \alpha_p + \frac{1}{2}\alpha_{l-1} + \frac{1}{2}\alpha_l, & \text{for } j = 1; \\ \sum_{p=1}^{j-1} p\alpha_p + \sum_{p=j}^{l-2} j\alpha_p + \frac{1}{2}j\alpha_{l-1} + \frac{1}{2}j\alpha_l, & \\ \qquad \text{for } j = 2, 3, \ldots, l-2; & \\ \frac{1}{2}\{\sum_{p=1}^{l-1} p\alpha_p + \frac{1}{2}l\alpha_{l-1} + (\frac{1}{2}l - 1)\alpha_l\}, & \text{for } j = l-1; \\ \frac{1}{2}\{\sum_{p=1}^{l-1} p\alpha_p + (\frac{1}{2}l - 1)\alpha_{l-1} + \frac{1}{2}l\alpha_l\}, & \text{for } j = l; \end{cases}$$

as

$$\mathbf{A}^{-1} = \begin{bmatrix} 1 & 1 & 1 & 1 & \ldots & 1 & \frac{1}{2} & \frac{1}{2} \\ 1 & 2 & 2 & 2 & \ldots & 2 & 1 & 1 \\ 1 & 2 & 3 & 3 & \ldots & 3 & \frac{3}{2} & \frac{3}{2} \\ 1 & 2 & 3 & 4 & \ldots & 4 & 2 & 2 \\ \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 1 & 2 & 3 & 4 & \ldots & (l-2) & \frac{1}{2}(l-2) & \frac{1}{2}(l-2) \\ \frac{1}{2} & 1 & \frac{3}{2} & 2 & \ldots & \frac{1}{2}(l-2) & \frac{1}{4}l & \frac{1}{4}(l-2) \\ \frac{1}{2} & 1 & \frac{3}{2} & 2 & \ldots & \frac{1}{2}(l-2) & \frac{1}{4}(l-2) & \frac{1}{4}l \end{bmatrix}.$$

(h) The compact real form of D_l is so$(2l)$.

(i) The adjoint representation for D_l for $l \geq 4$ is $\Gamma(\{0, 1, 0, \ldots, 0\})$ and for D_3 is $\Gamma(\{0, 1, 1\})$.

References

Adams, J. F. (1969). "Lectures on Lie Groups". W. A. Benjamin, New York.

Ado, I. D. (1947). *Uspeki Mat. Nauk (N.S.)* **2**, No. **6(22)**, 159-173. [Translation (1962): *Amer. Math. Soc. Trans. Series* 1, **9**, 308-327.]

Agrawala, V. K. (1980). *J. Math. Phys.* **21**, 1562-1565.

Akhiezer, N. I. and Glazman, I. M. (1961). "Theory of Linear Operators in Hilbert Space", Vol. I. Frederick Ungar, New York.

Altmann, S. L. (1957). *Proc. Camb. Phil. Soc.* **63**, 343-367.

Altmann, S. L. (1962). *Phil. Trans.* **A255**, 216-240.

Altmann, S. L. (1963). *Rev. Mod. Phys.* **35**, 641-645.

Altmann, S. L. and Cracknell, A. P. (1965). *Rev. Mod. Phys.* **37**, 19-32.

Baker, H. F. (1905). *Proc. London Math. Soc.* (2) **3**, 24-47.

Barut, A. O. and Raczka, R. (1977). "Theory of Group Representations and Applications". Polish Scientific Publishers, Warsaw.

Bateman, H. (1932). "Partial Differential Equations of Mathematical Physics". Cambridge U.P., Cambridge, England.

Behrends, R. E. (1968). *In* "Group Theory and its Applications" (Ed. E. M. Loebl), Vol. I, 541-627. Academic Press, Orlando, New York and London.

Behrends, R. E., Dreitlein, J., Fronsdal, C. and Lee, W. (1962). *Rev. Mod. Phys.* **34**, 1-40.

Bell, D. G. (1954). *Rev. Mod. Phys.* **26**, 311-320.

Berestetskii, V. B. (1965). *Soviet Phys. Uspekhi* **8**, 147-176.

Bertrand, J. (1966). *Ann. Inst. Henri Poincaré*, **5**, 235-256.

Biedenharn, L. C. and Louck, J. D. (1979a). "Angular Momentum in Quantum Mechanics". Addison-Wesley, Reading, Massachusetts.

Biedenharn, L. C. and Louck, J. D. (1979b). "The Racah-Wigner Algebra in Quantum Theory". Addison-Wesley, Reading, Massachusetts.

Bloch, F. (1928). *Z. Phys.* **52**, 555-600.

Born, M. and von Karman, T. (1912). *Phys. Z.* **13**, 297-309.

Bouckaert, L. P., Smoluchowski, R. and Wigner, E. P. (1936). *Phys. Rev.* **50**, 58-67.

Brennich, R. H. (1970). *Ann. Inst. Henri Poincaré* **13**, 137-161.

Burns, G. and Glazer, A. M. (1978). "Introduction to Space Groups for Solid State Scientists". Academic Press, Orlando, New York and London.

Butler, P. H. (1981). "Point Group Symmetry Applications, Methods and Tables". Plenum, New York.

Callaway, J. (1958). "Electron Energy Bands in Solids". *In* "Solid State Physics, Advances in Research and Applications", Vol. 7 (Eds. F. Seitz and D. Turnbull), 100-212. Academic Press, Orlando, New York and London.

Callaway, J. (1964). "Energy Band Theory". Academic Press, Orlando, New York and London.

Campbell, J. E. (1897a). *Proc. London Math. Soc.* (1) **28**, 381-390.

Campbell, J. E. (1897b). *Proc. London Math. Soc.* (1) **29**, 14-32.

Carruthers, P. (1966). "Unitary Symmetry of Strong Interactions". Wiley Interscience, New York.

Cartan, E. (1894). "Sur la Structure des Groupes de Transformations Finis et Continus". Thesis, Paris. [Reprint (1952): *In* "Oeuvres Completes", Partie I, Vol. I, 137-287. Vuibert, Paris.]

Cartan, E. (1914). *Ann. I'Ecole Norm. Sup. 3-eme serie* **31**, 263-355.

Cartan, E. (1929). *J. Math. Pure Appl.* **8**, 1-33.

Casimir, H. (1931). *Proc. R. Acad. Amstd.* **34**, 844-846.

Charap, J. M., Jones, R. B. and Williams, P. G. (1967). *Repts. Progr. Phys.* **30**, 227-283.

Chelikowsky, J. R. and Cohen, M. L. (1976). *Phys. Rev.* **B14**, 556-582.

Chevalley, C. (1946). "Theory of Lie Groups", Vol. 1. Princeton U.P., Princeton.

Cohen, E. R. (1974). "Tables of the Clebsch-Gordan Coefficients". North American Rockwell Science Center, Thousand Oaks, California.

Coleman, A. J. (1968). "Induced and Subduced Representations". *In* "Group Theory and its Applications" (Ed. E. M. Loebl), 57-118. Academic Press, Orlando, New York and London.

Condon, E. U. and Odabasi, H. (1980). "Atomic Structure". Cambridge U.P. Cambridge, England.

Condon, E. U. and Shortley, G H. (1935). "The Theory of Atomic Spectra". Cambridge U.P., Cambridge, England.

Cornwell, J. F. (1969). "Group Theory and Electronic Energy Bands in Solids". North Holland, Amsterdam.

Cornwell, J. F. (1971). *Phys. Status Solidi* **43(b)**, 763-767.

Cornwell, J. F. (1972). *Phys. Status Solidi* **52(b)**, 275-283.

Cornwell, J. F. (1984). "Group Theory in Physics". Vols. I and II. Academic Press, Orlando, New York and London.

de Franceschi, G. and Maiani, L. (1965). *Fortschr. Phys.* **13**, 279-384.

de Swart, J. J. (1963). *Rev. Mod. Phys.* **35**, 916-939.

de Swart, J. J. (1965). *Rev. Mod. Phys.* **37**, 326.

Donnay, J. D. H. and Nowacki, W. (1954). "Crystal Data". Geological Society of America, Memoir 60, New York.

Dynkin, E. B. (1947). *Uspeki. Mat. Nauk. (N.S.)* **2**, No. **4(20)**, 59-127 [Translation (1950): *Amer. Math. Soc. Trans. series* 1, **9**, 328-469.]

Dynkin, E. B. and Oniscik, A. L. (1955). *Uspeki. Mat. Nauk. (N.S.)* **10**, No. **4(66)**, 3-74. [Translation (1962): *Amer. Math. Soc. Trans. Series* 2, **21**, 119-192.]

Dyson, F. (1966). "Symmetry Groups in Nuclear and Particle Physics". W. A. Benjamin, New York.

Edmonds, A. R. (1957). "Angular Momentum in Quantum Mechanics". Princeton U.P., Princeton.

Emmerson, J. McL. (1972). "Symmetries in Particle Physics". Oxford U.P., Oxford.

Englefield, M. J. and King, R. C. (1980). *J. Phys.* **A13**, 2297-2317.

Fleming, W. (1977). "Functions of Several Variables", 2nd edition. Springer-Verlag, New York, Heidelberg and Berlin.

Fletcher, G. C. (1971). "The Electron Band Theory of Solids". North Holland, Amsterdam.

Freudenthal, H. and de Vries, H. (1969). "Linear Lie Groups". Academic Press, Orlando, New York and London.

Gantmacher, F. R. (1939a). *Rec. Math. (Mat. Sbornik) N.S.* **5(47)**, 101-144.

Gantmacher, F. R. (1939b). *Rec. Math. (Mat. Sbornik) N.S.* **5(47)**, 217-250.

Gantmacher, F. R. (1959). "The Theory of Matrices", Vol. 1. Chelsea Publishing, New York.

Gatto, R. (1964). *Nuovo Cimento Suppl.* **4**, 414-464.

Gel'fand, I. M. Minlos, R. A. and Shapiro, Z. Ya. (1963). "Representations of the Rotation and Lorentz Groups and their Applications". Pergamon Press, London.

Gell-Mann, M. (1953). *Phys. Rev.* **92**, 833-834.

Gell-Mann, M. (1961). California Institute of Technology Report CTSL-20, unpublished.

Gell-Mann, M. (1962). *Phys. Rev.* **125**, 1067-1084.

Gell-Mann, M. (1964). *Phys. Letts.* **8**, 214-215.

Gell-Mann, M. and Ne'eman, Y. (1964). "The Eightfold Way". W. A. Benjamin, New York.

Gell-Mann, M. and Pais, A. (1955). *In* "Proceedings of the 1954 Glasgow Conference on Nuclear and Meson Physics" (Eds. E. H. Bellamy and R. G. Moorhouse), 342-352. Pergamon Press, London and New York.

Glashow, S. L. (1980). *Rev. Mod. Phys.* **52**, 539-543.

Goldstone, J. (1961). *Nuovo Cimento* **19**, 154-164.

Goldstone, J., Salam, A. and Weinberg, S. (1962). *Phys. Rev.* **127**, 965-970.

Goto, M. and Grosshans, F. D. (1978). "Semi-simple Lie Algebras". Marcel Dekker, New York and Basel.

Gourdin, M. (1967). "Unitary Symmetries". North Holland, Amsterdam.

Gruber, B. and O'Raifeartaigh, L. (1964). *J. Math. Phys.* **5**, 1796-1804.

Haar, A. (1933). *Ann. Math.* **34**, 147-169.

Halmos, P. R. (1950). "Measure Theory". D. Van Nostrand, New York.

Halpern, F. R. (1968). "Special Relativity and Quantum Mechanics". Prentice-Hall, Englewood Cliffs, New Jersey.

Hausdorff, F. (1906). *Leipz. Ber.* **58**, 19-48.

Helgason, S. (1962). "Differential Geometry and Symmetric Spaces". Academic Press, Orlando, New York and London.

Helgason, S. (1978). "Differential Geometry, Lie Groups, and Symmetric Spaces". Academic Press, Orlando, New York and London.

Henry, N. F. M. and Lonsdale, K. (1965). *International Tables for X-ray Crystallography*, Vol. I. International Union of Crystallography, Kynoch Press, Birmingham, England.

Herring, C. (1937). *Phys. Rev.* **52**, 365-373.

Hewitt, E. and Ross, K. A. (1963). "Abstract Harmonic Analysis", Vol. I. Springer-Verlag, Berlin.

Higgs, P. W. (1964a). *Phys. Letts.* **12**, 132-133.

Higgs, P. W. (1964b). *Phys. Rev. Letts.* **13**, 508-509.

Higgs, P. W. (1966). *Phys. Rev.* **145**, 1156-1163.

Howarth, D. J. and Jones, H. (1952). *Proc. Phys. Soc.* **A65**, 355-368.

Humphreys, J. E. (1972). "Introduction to Lie Algebras and Representation Theory". Springer-Verlag, New York, Heidelberg and Berlin.

Inönü, E. and Wigner, E. P. (1952). *Nuovo Cimento.* **9**, 705-718.

Jacobson, N. (1962). "Lie Algebras". Interscience, New York.

Killing, W. (1888). *Math. Ann.* **31**, 252-290.

Killing, W. (1889a). *Math. Ann.* **33**, 1-48.

Killing, W. (1889b). *Math. Ann.* **34**, 57-122.

Killing, W. (1890). *Math. Ann.* **36**, 161-189.

Klimyk, A. U. (1971). *Teor. and Mat. Fiz. (USSR)* **8**, 55-60.

Klimyk, A. U. (1972). *Teor. and Mat. Fiz. (USSR)* **13**, 327-342. [Translation (1972): *Theor. and Math. Phys.* **13**, 1171-1182.]

Klimyk, A. U. (1975). *Repts. Math. Phys.* **7**, 153-166.

Kokkedee, J. J. J. (1969). "The Quark Model". W. A. Benjamin, New York.

Koster, G. F., Dimmock, J. O., Wheeler, R. E. and Statz, H. (1964). "Properties of the Thirty-two Point Groups". M.I.T. Press, Cambridge, Massachusetts.

Koster, G. F. (1957). *In* "Solid State Physics, Advances in Research and Applications" (Eds. F. Seitz and D. Turnbull), Vol. 5,173-256. Academic Press, Orlando, New York and London.

Kudryavtseva, N. V. (1967). *Fiz. Tverd. Tela* **9**, 2364-2368. [Translation (1968): *Soviet Physics, Solid State* **9**, 1850-1853.]

Lichtenberg, D. B. (1978). "Unitary Symmetry and Elementary Particles". Academic Press, Orlando, New York and London.

Lipsman, R. L. (1974). "Group Representations", Lecture Notes in Mathematics, Vol. 388. Springer-Verlag, Berlin

Lomont, J. S. (1959). "Applications of Finite Groups". Academic Press, Orlando, New York and London.

London, G. W. (1964). *Fortschr. Phys.* **12**, 643-666.

Loomis, L. H. (1953). "An Introduction to Abstract Harmonic Analysis". D. Van Nostrand, Princeton.

Luehrmann, A. W. (1968). *Adv. Phys.* **17**,1-77.

Mackey, G. W. (1963). *Bull. Amer. Math. Soc.* **69**, 628-686.

Mackey, G. W. (1968). "Induced Representation of Groups and Quantum Mechanics". W. A. Benjamin, New York.

Mackey, G. W. (1976). "The Theory of Unitary Group Representations". University of Chicago Press, Chicago and London.

Mathews, P. T. (1967). *In* "High Energy Physics" (Ed. E. H. Burhop), Academic Press, Orlando, New York and London.

Miller, W. (1964). *Commun. Pure Appl. Math.* **17**, 527-540.

Moody, R.V., Patera, J. and Rand, D. (1996) "SimpLie^{TM}" software. Centre de Recherches Mathematiques, Montreal.

Naimark, M. A. (1957). *Amer. Math. Soc. Trans. Series 2*, **6**, 379-458. [Original (1954): *Uspeki Mat. Nauk (N.S.)* **9**, No. **4(62)**, 19-93.]

Naimark, M. A. (1964). "Linear Representations of the Lorentz Group". Pergamon Press, London.

Nakano, T. and Nishijima, K. (1953). *Progr. Theor. Phys.* **10**, 581-582.

Ne'eman, Y. (1961). *Nucl. Phys.* **26**, 222-269.

Ne'eman, Y. (1965). *In* "Progress in Elementary Particle and Cosmic Ray Physics" (Eds. J. G. Wilson and S. A. Wouthysen), 69-118. North Holland, Amsterdam.

Niederer, U. H. and O'Raifeartaigh, L. (1974a). *Forts. der Physik* **22**, 111-129.

Niederer, U. H. and O'Raifeartaigh, L. (1974b). *Forts. der Physik* **22**, 131-157.

Nishijima, K. (1954). *Progr. Theor. Phys.* **12**, 107-108.

Okubo, S. (1977). *J. Math. Phys.* **18**, 2382-2394.

O'Raifeartaigh, L. (1968). *In* "Group Theory and its Applications" (Ed. E. M. Loebl), Vol. I, 469-540. Academic Press, Orlando, New York and London.

Pais, V. (1952). *Phys. Rev.* **86**, 663-672.

Peter, F. and Weyl, H. (1927). *Math. Ann.* **97**, 737-755.

Phillips, J. C. (1956). *Phys. Rev.* **104**, 1263-1277.

Pincherle, L. (1960). *Rep. Progr. Phys.* **23**, 355-394.

Pincherle, L. (1971). "Electronic Energy Bands in Solids". McDonald, London.

Pontrjagin, L.S. (1946). "Topological Groups". Princeton U.P., Princeton.

Pontrjagin, L.S. (1986). "Topological Groups". *In* "L.S.Pontrjagin, Selected Works" Vol. 2. Gordon and Breach, New York.

Price, J. F. (1977). "Lie Groups and Compact Groups". Cambridge U.P., Cambridge, England.

Racah, G. (1942). *Phys. Rev.* **62**, 438-462.

Racah, G. (1950). *Rend. Lincei* **8**, 108-112.

Racah, G. (1951). *Ergebnisse der Exacten Naturwissenschaften*, **37**, 28-84.

Rashba, E. I. (1959). *Fiz. Tvend. Tela* **1**, 407-421. [Translation (1959): *Soviet Phys. Solid State* **1**, 368-380.]

Reitz, J. R. (1955). *In* "Solid State Physics, Advances in Research and Applications", Vol. 1 (Eds. F. Seitz and D. Turnbull), 1-95. Academic Press, Orlando, New York and London.

Riesz, F. and Sz.-Nagy, B. (1956). "Functional Analysis". Blackie and Son, London and Glasgow.

Rose, M. E. (1957). "Elementary Theory of Angular Momentum". J. Wiley and Sons, New York.

Rotman, J. J. (1965). "The Theory of Groups". Allyn and Bacon, Boston.

Sagle, A. A. and Walde, R. E. (1973). "Introduction to Lie Groups and Lie Algebras". Academic Press, Orlando, New York and London.

Salam, A. (1980). *Rev. Mod. Phys.* **52**, 525-538.

Samelson, H. (1969). "Notes on Lie Algebras". Van Nostrand Reinhold, New York.

Schiff, L. I. (1968). "Quantum Mechanics". McGraw-Hill, New York and London.

Schlosser, H. (1962). *J. Phys. Chem. Solids* **23**, 963-969.

Schönfliess, A. (1923). "Theorie der Kristallstruktur". Bomtraeger, Berlin.

Schwinger, J. (1952). "On Angular Momentum". U.S. Atomic Energy Commission, NYO-3071.

Shaw, R. (1955). "The Problem of Particle Types and Other Contributions to the Theory of Elementary Particles". Ph.D. Thesis, Cambridge University, unpublished.

Sheka, V. I. (1960). *Fiz. Tvend. Tela*, **2**, 1211-1219. [Translation (1960): *Soviet Phys. Solid State* **2**, 1096-1104.]

Shephard, G. C. (1966). "Vector Spaces of Finite Dimension". Oliver and Boyd, Edinburgh and London.

Shubnikov, A. V. and Koptsik, V. A. (1974) "Symmetry in Science and Art". Plenum, New York.

Simmons, G F (1963). "Topology and Modern Analysis". McGraw-Hill, New York and London.

Smorodinsky, Ya. A. (1965). *Soviet Phys. Uspekhi* **7**, 637-655.

Stein, E. M. (1965). *In* "High Energy Physics and Elementary Particles" (Ed. A. Salam), 563-584. International Atomic Energy, Vienna.

van den Broek, P. M. and Cornwell, J. F. (1978). *Phys. Stat. Sol.* **90(b)**, 211-224.

van Hove, L. (1953). *Phys. Rev.* **89**, 1189-1193.

Varadarajan, V. S. (1974). "Lie Groups, Lie Algebras, and their Representations". Prentice-Hall, Englewood Cliffs, New Jersey.

Voisin, J. (1965a). *J. Math. Phys.* **6**, 1519-1529.

Voisin, J. (1965b). *J. Math. Phys.* **6**, 1822-1832.

Voisin, J. (1966). *J. Math. Phys.* **7**, 2235-2237.

von der Lage, F. C. and Bethe, H. A. (1947). *Phys. Rev.* **71**, 612-622.

Warner, F. W. (1971). "Foundations of Differentiable Manifolds and Lie Groups". Scott, Foreman and Co. Glenview, Illinois and London.

Weinberg, S. (1980). *Rev. Mod. Phys.* **52**, 515-523.

Weyl, H. (1925). *Math. Zeits.* **23**, 271-309.

Weyl, H. (1926a). *Math. Zeits.* **24**, 328-376.

Weyl, H. (1926b). *Math. Zeits.* **24**, 377-395.

Wigner, E. P. (1939). *Ann. Math.* **40**, 149-204.

Wigner, E. P. (1959). "Group Theory and its Application to the Quantum Mechanics of Atomic Spectra". Academic Press, Orlando, New York and London.

Wondratschek, H. and Neubuser, J. (1967). *Acta. Cryst.* **23**, 349-352.

Wood, J. H. (1962). *Phys. Rev.* **126**, 517-527.

Wybourne, B. G. (1970). "Symmetry Principles and Atomic Spectroscopy". J. Wiley and Sons, New York.

Wyckoff, R. W. G. (1963). "Crystal Structures 1". Interscience, New York.

Wyckoff, R. W. G. (1964). "Crystal Structures 2". Interscience, New York.

Wyckoff, R. W. G. (1965). "Crystal Structures 3". Interscience, New York.

Yang, C. N. and Mills, R. L. (1954). *Phys. Rev.* **96**, 191-195.

Zweig, G. (1964). *CERN Repts.* TH 401 and TH 402.

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